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SOLUBILITY DATA SERIES

Volume 38

HYDROCARBONS WITH WATER AND SEAWATER

Part II: Hydrocarbons C8 to C36

SOLUBILITY DATA SERIES

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SOLUBILITY DATA SERIES

Editor-in-Chief A.S. KERTES

Volume 38

HYDROCARBONS WITH WATER AND SEAWATER

Part II: Hydrocarbons C₈ to C₃₆

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FOREWORD

If the knowledge is undigested or simply wrong, more is not better

How to communicate and disseminate numerical data effectively in chemical science and technology has been a problem of serious and growing concern to IUPAC, the International Union of Pure and Applied Chemistry, for the last two decades. The steadily expanding volume of numerical information, the formulation of new interdisciplinary areas in which chemistry is a partner, and the links between these and existing traditional subdisciplines in chemistry, along with an increasing number of users, have been considered as urgent aspects of the information problem in general, and of the numerical data problem in particular.

Among the several numerical data projects initiated and operated by various IUPAC commissions, the Solubility Data Project is probably one of the most ambitious ones. It is concerned with preparing a comprehensive critical compilation of data on solubilities in all physical systems, of gases, liquids and solids. Both the basic and applied branches of almost all scientific disciplines require a knowledge of solubilities as a function of solvent, temperature and pressure. Solubility data are basic to the fundamental understanding of processes relevant to agronomy, biology, chemistry, geology and oceanography, medicine and pharmacology, and metallurgy and materials science. Knowledge of solubility is very frequently of great importance to such diverse practical applications as drug dosage and drug solubility in biological fluids, anesthesiology, corrosion by dissolution of metals, properties of glasses, ceramics, concretes and coatings, phase relations in the formation of minerals and alloys, the deposits of minerals and radioactive fission products from ocean waters, the composition of ground waters, and the requirements of oxygen and other gases in life support systems.

The widespread relevance of solubility data to many branches and disciplines of science, medicine, technology and engineering, and the difficulty of recovering solubility data from the literature, lead to the proliferation of published data in an ever increasing number of scientific and technical primary sources. The sheer volume of data has overcome the capacity of the classical secondary and tertiary services to respond effectively.

While the proportion of secondary services of the review article type is generally increasing due to the rapid growth of all forms of primary literature, the review articles become more limited in scope, more specialized. The disturbing phenomenon is that in some disciplines, certainly in chemistry, authors are reluctant to treat even those limited-in-scope reviews exhaustively. There is a trend to preselect the literature, sometimes under the pretext of reducing it to manageable size. The crucial problem with such preselection - as far as numerical data are concerned - is that there is no indication as to whether the material was excluded by design or by a less than thorough literature search. We are equally concerned that most current secondary sources, critical in character as they may be, give scant attention to numerical data.

On the other hand, tertiary sources - handbooks, reference books and other tabulated and graphical compilations - as they exist today are comprehensive but, as a rule, uncritical. They usually attempt to cover whole disciplines, and thus obviously are superficial in treatment. Since they command a wide market, we believe that their service to the advancement of science is at least questionable. Additionally, the change which is taking place in the generation of new and diversified numerical data, and the rate at which this is done, is not reflected in an increased third-level service. The emergence of new tertiary literature sources does not parallel the shift that has occurred in the primary literature. With the status of current secondary and tertiary services being as briefly stated above, the innovative approach of the *Solubility Data Project* is that its compilation and critical evaluation work involve consolidation and reprocessing services when both activities are based on intellectual and scholarly reworking of information from primary sources. It comprises compact compilation, rationalization and simplification, and the fitting of isolated numerical data into a critically evaluated general framework.

The Solubility Data Project has developed a mechanism which involves a number of innovations in exploiting the literature fully, and which contains new elements of a more imaginative approach for transfer of reliable information from primary to secondary/tertiary sources. The fundamental trend of the Solubility Data Project is toward integration of secondary and tertiary services with the objective of producing in-depth critical analysis and evaluation which are characteristic to secondary services, in a scope as broad as conventional tertiary services.

Fundamental to the philosophy of the project is the recognition that the basic element of strength is the active participation of career scientists in it. Consolidating primary data, producing a truly critically-evaluated set of numerical data, and synthesizing data in a meaningful relationship are demands considered worthy of the efforts of top scientists. Career scientists, who themselves contribute to science by their involvement in active scientific research, are the backbone of the project. The scholarly work is commissioned to recognized authorities, involving a process of careful selection in the best tradition of IUPAC. This selection in turn is the key to the quality of the output. These top experts are expected to view their specific topics dispassionately, paying equal attention to their own contributions and to those of their peers. They digest literature data into a coherent story by weeding out what is wrong from what is believed to be right. To fulfill this task, the evaluator must cover all relevant open literature. No reference is excluded by design and every effort is made to detect every bit of relevant primary source. Poor quality or wrong data are mentioned and explicitly disqualified as such. In fact, it is only when the reliable data are presented alongside the unreliable data that proper justice can be done. The user is bound to have incomparably more confidence in a succinct evaluative commentary and a comprehensive review with a complete bibliography to both good and poor data.

It is the standard practice that the treatment of any given solute-solvent system consists of two essential parts: I. Critical Evaluation and Recommended Values, and II. Compiled Data Sheets.

The Critical Evaluation part gives the following information:

- (i) a verbal text of evaluation which discusses the numerical solubility information appearing in the primary sources located in the literature. The evaluation text concerns primarily the quality of data after consideration of the purity of the materials and their characterization, the experimental method employed and the uncertainties in control of physical parameters, the reproducibility of the data, the agreement of the worker's results on accepted test systems with standard values, and finally, the fitting of data, with suitable statistical tests, to mathematical functions;
- (ii) a set of recommended numerical data. Whenever possible, the set of recommended data includes weighted average and standard deviations, and a set of smoothing equations derived from the experimental data endorsed by the evaluator;
- (iii) a graphical plot of recommended data.

The Compilation part consists of data sheets of the best experimental data in the primary literature. Generally speaking, such independent data sheets are given only to the best and endorsed data covering the known range of experimental parameters. Data sheets based on primary sources where the data are of a lower precision are given only when no better data are available. Experimental data with a precision poorer than considered acceptable are reproduced in the form of data sheets when they are the only known data for a particular system. Such data are considered to be still suitable for some applications, and their presence in the compilation should alert researchers to areas that need more work.

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The typical data sheet carries the following information:

- (i) components definition of the system their names, formulas and Chemical Abstracts registry numbers;
- (ii) reference to the primary source where the numerical information is reported. In cases when the primary source is a less common periodical or a report document, published though of limited availability, abstract references are also given;
- (iii) experimental variables;
- (iv) identification of the compiler;
- (v) experimental values as they appear in the primary source. Whenever available, the data may be given both in tabular and graphical form. If auxiliary information is available, the experimental data are converted also to SI units by the compiler.

Under the general heading of Auxiliary Information, the essential experimental details are summarized:

- (vi) experimental method used for the generation of data;
- (vii) type of apparatus and procedure employed;
- (viii) source and purity of materials;
- (ix) estimated error;
 - (x) references relevant to the generation of experimental data as cited in the primary source.

This new approach to numerical data presentation, formulated at the initiation of the project and perfected as experience has accumulated, has been strongly influenced by the diversity of background of those whom we are supposed to serve. We thus deemed it right to preface the evaluation/compilation sheets in each volume with a detailed discussion of the principles of the accurate determination of relevant solubility data and related thermodynamic information.

Finally, the role of education is more than corollary to the efforts we are seeking. The scientific standards advocated here are necessary to strengthen science and technology, and should be regarded as a major effort in the training and formation of the next generation of scientists and engineers. Specifically, we believe that there is going to be an impact of our project on scientific-communication practices. The quality of consolidation adopted by this program offers down-to-earth guidelines, concrete examples which are bound to make primary publication services more responsive than ever before to the needs of users. The self-regulatory message to scientists of the early 1970s to refrain from unnecessary publication has not achieved much. A good fraction of the literature is still cluttered with poor-quality articles. The Weinberg report (in 'Reader in Science Information', ed. J. Sherrod and A. Hodina, Microcard Editions Books, Indian Head, Inc., 1973, p. 292) states that 'admonition to authors to restrain themselves from premature, unnecessary publication can have little effect unless the climate of the entire technical and scholarly community encourages restraint... We think that projects of this kind translate the climate into operational terms by exerting pressure on authors to avoid submitting low-grade material. The type of our output, we hope, will encourage attention to quality as authors will increasingly realize that their work will not be suited for permanent retrievability unless it meets the standards adopted in this project. It should help to dispel confusion in the minds of many authors of what represents a permanently useful bit of information of an archival value, and what does not.

If we succeed in that aim, even partially, we have then done our share in protecting the scientific community from unwanted and irrelevant, wrong numerical information.

A. S. Kertes

PREFACE

This volume presents solubility data for binary systems in which one component is a hydrocarbon containing 8 to 36 carbon atoms and the second component is water, heavy water or seawater. Other volumes in this series either presently available or in preparation present analogous data for other hydrocarbons. The interested reader should consult the Solubility Data Series list of volume titles on page 561. For this volume seawater has been defined as, "all natural waters, synthetic seawater and aqueous solutions in which sodium chloride predominates."

A variety of units for the expression of solubility has appeared in the primary literature. For the purpose of comparison the compilers of this volume have, so far as possible, expressed all original results in terms of mass percent and mole fraction as well as the units presented by the original investigators. Where such conversions have been made, they are clearly attributed to the compiler and the source of any data not provided by the original investigators (such as hydrocarbon or seawater density) is specified. Definitions of mass percent and mole fraction as well as their relationship to other common measures of solubility are given in the Introduction to this volume.

The expression of the solubility of a hydrocarbon in natural seawater on a mole fraction basis presents special difficulties since the composition of seawater is not fully known and somewhat variable. However, the uncertainty introduced by this factor is generally less than 3%, smaller than the measurement uncertainty associated with many of these data. Some of the data for hydrocarbon solubility in seawater have been presented in terms of the Setschenow (also transliterated Sechenov and Setchenoff) equation. A thorough discussion, "The Sechenov Salt Effect Parameter", is presented in Volume 10 of this series (pp. xxix-xliii).

By far the most common approach to the measurement of solubility in hydrocarbon/water systems has been to prepare a saturated solution and then to analytically determine the concentration of the less abundant component. In these systems of low solubility the careful preparation of saturated solutions is critically important. The presence of only a small amount of the minor component in the form of colloidal droplets can significantly influence the solubility results obtained. This can lead to major positive systematic errors. Unfortunately, lack of experimental detail in some published reports makes these errors extremely difficult to evaluate. Users of this volume are advised to be aware of this potential source of error, especially for systems where only one or a few measurements have been reported or when solubilities are very low. Another approach to evaluating solubility data in these systems is to determine whether a particular result fits into a "reasonable" trend for a series of related compounds. While this approach undoubtedly has qualitative value, it must be used with caution. For instance, the solubilities of anthracene and phenanthrene differ by about a factor of 20; a fact that is supported by careful experimentation but not by "reasonable" inference.

Most measurements of hydrocarbon/water solubility have been made within the temperature range considered "room temperature" (275-300 K). In many reports system pressure is unspecified but can be assumed to be approximately 100 kPa (1 atm). Some measurements at elevated temperatures have been in sealed tubes. Generally the system pressure for these measurements is not known. For most purposes this lack of specification of system pressure is not important since hydrocarbon/water solubilities do not vary strongly with pressure.

This volume is the result of a careful search of the chemical literature. The goal of that search was to include all published data for the systems indicated in the title. Each evaluation includes a closing date for the literature search of that system, November 1981 or later. In spite of these efforts, some published measurements may have been missed. The editor will appreciate having his attention brought to any omitted source of solubility data for inclusion in future volumes.

The compilation and critical evaluation of solubility data presented here was a group effort. Each participant brought an individual style to the work. The editor's goal was to ensure that all text is simple, unambiguous English; not to attempt stylistic uniformity. Finally the editor wishes to acknowledge the dedicated efforts of the compilers, evaluators and reviewers whose efforts have resulted in this volume, and especially to thank Mauricette Nicpon, Sheila Chapin and Bronwyn Airey for final typing.

David Shaw

INTRODUCTION TO THE SOLUBILITY OF LIQUIDS IN LIQUIDS

The Solubility Data Series is made up of volumes of comprehensive and critically evaluated solubility data on chemical systems in clearly defined areas. Data of suitable precision are presented on data sheets in a uniform format, preceded for each system by a critical evaluation if more than one set of data is available. In those systems where data from different sources agree sufficiently, recommended values are proposed. In other cases, values may be described as "tentative", "doubtful" or "rejected".

This volume is primarily concerned with liquid-liquid systems, but related gas-liquid and solid-liquid systems are included when it is logical and convenient to do so. Solubilities at elevated and low temperatures and at elevated pressures may be included, as it is considered inappropriate to establish artificial limits on the data presented.

For some systems the two components are miscible in all proportions at certain temperatures or pressures, and data on miscibility gap regions and upper and lower critical solution temperatures are included where appropriate and if available.

TERMINOLOGY

In this volume a mixture (1,2) or a solution (1,2) refers to a single liquid phase containing components 1 and 2, with no distinction being made between solvent and solute.

The *solubility* of a substance 1 is the relative proportion of 1 in a mixture which is saturated with respect to component 1 at a specified temperature and pressure. (The term "saturated" implies the existence of equilibrium with respect to the processes of mass transfer between phases).

QUANTITIES USED AS MEASURES OF SOLUBILITY

<u>Mole fraction</u> of component 1, x_1 or x(1):

$$x_{1} = n_{1} / \sum_{i=1}^{n} i = \frac{m_{1} / M_{1}}{\sum_{i=1}^{n} (m_{i} / M_{i})}$$

where n_i is the amount of substance (number of moles) of component i, m_i is the mass of substance i, and M_i is its molar mass.

<u>Mole per cent</u> of component 1 is $100x_1$.

<u>Mass fraction</u> of component 1, w_1

$$w_1 = m_1 / \sum_{i=1}^{\infty} i$$

where m_i is the mass of component i.

<u>Mass percent</u> of component 1 is $100w_1$, and may be described as g(1)/100 gsln which makes it clear that it is mass percent of solute relative to solution and not solvent. The equivalent terms "weight fraction" and "weight percent" are not used. The mole fraction solubility is related to the mass fraction solubility in a binary system by

$$x_{1} = \frac{w_{1}/M_{1}}{w_{1}/M_{1} + (1 - w_{1})/M_{2}}$$

<u>Amount-of-substance concentration</u> of component 1 in a solution of volume V,

$$c_1 = n_1 / v$$

is expressed in units of mol dm^{-3} . The terms "molarity" and "molar" and the unit symbol M are not used.

<u>Mass ratio</u> is occasionally used in a two-component solution in the form g(1)/g(2), mg(1)/g(2), etc. The term "part per million" (ppm) is not used, but may be expressed as $mg(1)/kg \ sln$.

<u>Molality</u> of component 1 in component 2 is often used in solid-liquid systems, defined $m_1 = n_1/n_2 M_2$, with units mol kg⁻¹, but is not used in liquid-liquid systems where the distinction between "solute" 1 and "solvent" 2 is inappropriate. The term molality alone is inadequate, and the unit (mol kg⁻¹, mmol kg⁻¹) must be stated.

Mole fractions and mass fractions are appropriate to either the "mixture" or the "solution" point of view; the other quantities are appropriate to the solution point of view only.

ORDERING OF SYSTEMS

It is necessary to establish a method of ordering chemical compounds, to be used for the lists of saturating components which define each chemical system. This order is also used for ordering systems within volumes.

The systems are ordered first on the basis of empirical formula according to the Hill system (ref 2). The organic compounds within each Hill formula are ordered as follows:

- (i) by degree of unsaturation (e.g. cycloalkene, diene, alkyne, cycloalkane, alkane), then
- (ii) by order of increasing chain length in the parent hydrocarbon, then
- (iii) by order of increasing chain length of hydrocarbon branches, then
- (iv) numerically by position of unsaturation, then
- (v) numerically by position of substitution, then
- (vi) alphabetically by IUPAC name.

For example,

с ₅ н ₈	cyclopentene 2-methyl-1,3-butadiene 1,4-pentadiene 1-pentyne
C ₅ H ₁₀	cyclopentane 3-methyl-1-butene 2-methyl-2-butene 1-pentene 2-pentene
C ₅ H ₁₂	2,2-dimethylpropane 2-methylbutane pentane
с ₅ н ₁₂ о	2,2-dimethyl-1-propanol 2-methyl-1-butanol 2-methyl-2-butanol 3-methyl-1-butanol 3-methyl-2-butanol 1-pentanol 2-pentanol 3-pentanol

Introduction

C₆H₁₂0 cyclohexanol 4-methyl-1-penten-3-ol 1-hexen-3-ol 4-hexen-3-ol C₁₈H₁₂ benzanthracene chrysene naphthacene triphenylene

Deuterated compounds immediately follow the corresponding ¹H compounds.

GUIDE TO THE COMPILATIONS AND EVALUATIONS

The format used for the compilations and evaluations has been discussed in the Foreword. Additional information on the individual sections of each sheet is now provided in the following.

"Components". Each component is listed by IUPAC name (ref 1), chemical formula according to the Hill system, and Chemical Abstracts Registry Number. Also included are trivial name or names if appropriate.

"Original Measurements". References are expressed in "Chemical Abstracts" style, journal names being abbreviated, and if necessary transliterated, in the forms given by the "Chemical Abstracts Service Source Index" (CASSI).

"Variables". Ranges of variations of temperature, pressure, etc. are indicated here.

"Prepared by". The compiler is named here.

"Experimental Values". Components are described as (1) and (2), as defined in "Components". The experimental data are presented in the units used in the original paper. Thus the temperature is expressed $t/^{\circ}C$ or $T/^{\circ}F$ as in the original, and conversion to T/K is made only in the critical evaluation. However, the authors's units are expressed according to IUPAC recommendations (ref 3,4) as far as possible.

In addition, compiler-calculated values of mole fractions and/or mass percent are included if the original data do not use these units. 1975 or 1977 atomic weights (ref 5) are used in such calculations. When appropriate, conversions from concentrations to mole fractions are included in the compilation sheets, with the values and sources of the densities being quoted and referenced.

Details of smoothing equations (with limits) are included if they are present in the original publication and if the temperature or pressure ranges are wide enough to justify this procedure.

Errors in calculations, fitting equations, etc. are noted, and where possible corrected. Material inserted by the compiler is identified by the word "compiler" in parentheses.

The precision of the original data is preserved when derived quantities are calculated, if necessary by the inclusion of one additional significant figure.

"Method". An outline of the method is presented, reference being made to sources of further detail if these are cited in the original paper. "Chemical Abstracts" abbreviations are often used in this text.

"Source and Purity of Materials". For each component, referred to as (1) or (2), the following information (in this order and in abbreviated form) is provided if it is available in the original paper:

source and specification method of preparation properties degree of purity. "Estimated Error". If this information was omitted by the authors, and if the necessary data are available in the paper, the compilers have attempted to estimate errors (identified by "compiler" in parentheses) from the internal consistency, the type of apparatus, and other relevant information. Methods used by the compilers for reporting estimating errors are based on the papers by Ku and Eisenhart (ref 6).

"References". These are the references (usually cited in the original paper) which the compiler considers particularly useful in discussing the method and material.

"Evaluator". The information provided here is the name of the evaluator, the evaluator's affiliation, and the date of the evaluation.

"Critical Evaluation". The evaluator aims, to the best of his or her ability, to check that the compiled data are correct, to assess their reliability and quality, to estimate errors where necessary, and to recommend numerical values. The summary and critical review of all the data supplied by the compiler include the following information:

(a) *Critical text*. The evaluator produces a text evaluating *all* the published data for the particular system being discussed, reviewing their merits or shortcomings. Only published data are considered, and even some of the published data may only be referred to in this text if it is considered that inclusion of a data compilation sheet is unjustified.

(b) Fitting equations. If the use of a smoothing equation is justifiable, the evaluator may provide an equation representing the solubility as a function of the variables reported in the compilation sheets, stating the limits within which it should be used.

(c) Recommended values. Data are recommended if the results of at least two independent experimental groups are available and are in good agreement, and if the evaluator has no doubt as to the adequacy and reliability of the experimental and computational procedures used.

Data are reported as *tentative* if only one set of measurements is available, or if the evaluator is uncertain of the reliability of some aspect of the experimental or computational method but judges that it should cause only minor error, or if the evaluator considers some aspect of the computational or experimental method undesirable but believes the data to have some value in those instances when an approximate value of the solubility is needed.

Data determined by an inadequate method or under ill-defined conditions is *rejected*, the reference being included in the evaluation together with a reason for its rejection by the evaluator.

(d) *References*. All pertinent references are listed here, including all those publications appearing in the accompanying compilation sheets and also those which have been rejected and not compiled.

(e) Units. The final recommended values are reported in SI units (ref 3).

Continuation Sheets. These are used for both compilations and evaluations, and include sections listing the "Components" and also the "Original Measurement" or "Evaluator". Compilation continuation sheets may include a section headed "Comments and/or Additional Data". REFERENCES

- 1. Rigaudy, J.; Klesney, S.P. Nomenclature of Organic Chemistry (IUPAC), ("The Blue Book"), Pergamon, Oxford, <u>1979</u>.
- 2. Hill, E.A. J. Am. Chem. Soc. 1900, 22, 478.
- 3. Whiffen, D.H., ed. Manual of Symbols and Terminology for Physicochemical Quantities and Units (IUPAC), ("The Green Book"), Pergamon, Oxford, <u>1979</u>; Pure Appl. Chem. <u>1979</u>, 51, 1.
- 4. McGlashan, M.L. *Physicochemical Quantities and Units*, 2nd ed. Royal Institute of Chemistry, London, <u>1971</u>.
- 5. IUPAC Commission on Atomic Weight, Pure Appl. Chem. <u>1976</u>, 47, 75; <u>1979</u>, 51, 405.
- Ku, H.H., and Eisenhart, C., in Ku, H.H., ed. Precision Measurement and Calibration, NBS Special Publication 300, Vol. 1, Washington D.C., <u>1969</u>.

THE PHASE BEHAVIOR OF WATER AND HYDROCARBON SYSTEMS

C. L. Young Department of Physical Chemistry Parkville, Victoria, 3052 Australia

In order to understand solubility in hydrocarbon + water systems at high pressure it is desirable to be aware of the various types of fluid phase equilibria possible in binary mixtures. Fluid phase equilibria of binary mixtures are conveniently discussed in terms of the classification proposed by Scott and van Konynenburg¹⁻⁴. They proposed that the phase behavior of binary mixtures could be classified into six broad groups. They found that five groups could be predicted using the van der Waals equation of state. The sixth class, which could not be predicted by the van der Waals equation, arises only in aqueous mixtures. The classification is most easily understood in terms of the pressure-temperature projection of the pressure-temperature-composition diagram. The six types of phase behavior are represented schematically in fig. 1. Only the "general" characteristics of the type of phase behavior can be understood from the diagrams given below. In practice solid phases often complicate the diagrams.

Type I. The phase diagram has a simple continuous gas-liquid critical locus with or without azeotropy.

Type II. The phase diagram is as for type I but with the addition of a three phase (liquid-liquid-gas) line ending at an upper critical end point, UCEP, and a (liquid-liquid) critical line starting from the UCEP and rapidly approaching high pressures. This type can occur with or without azeotropy.

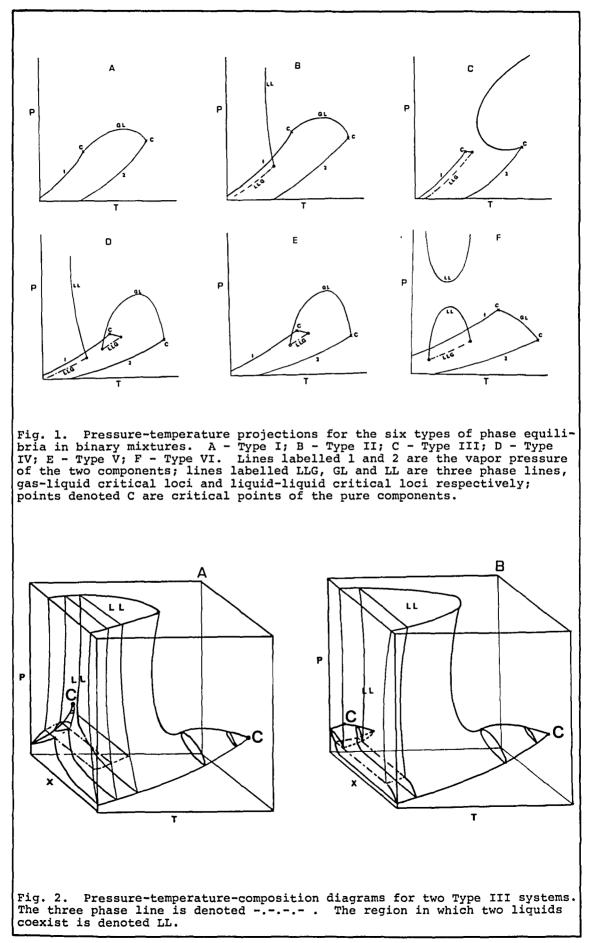
Type III. This phase diagram has two distinct critical lines, one starts at the critical point of the pure component with the higher critical temperature but never approaches the critical point of the other component moving rapidly to high pressures. The other critical line starts at the critical point of the component with the lower critical temperature and meets a three phase (liquid-liquid-gas) line in an UCEP. The three phase line may be between the vapor pressure curves of the two components (as shown in fig. 1C) or may be above the vapor pressure curves of both components. There are several subgroups in type III behavior depending on whether there is a heteroazeotrope or not and on the shape of the critical line starting at the critical point with the higher temperature.

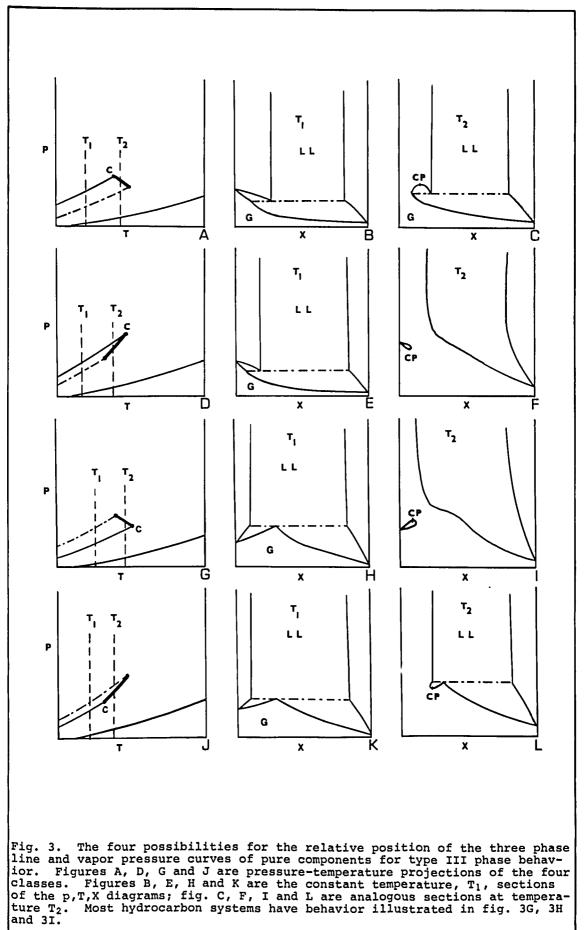
Type IV. This phase diagram has three distinct critical loci, one of which (the liquid-liquid critical line) starts at an UCEP on a three phase (liquid-liquid-gas) line and moves rapidly to higher pressures. The second line starts at the critical point of the component with the lower critical temperature and ends at an UCEP on a three phase line. The third line starts at the critical point of the other component and ends in a lower critical end point, LCEP, on the same three phase line as the second critical line.

Type V. This type is the same as type IV but without the liquidliquid critical line and the three phase line at lower temperatures.

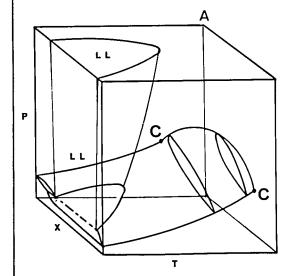
Type VI. This type of phase behavior is characterized by a continuous critical locus between the critical point of the two pure components. However, at lower temperatures there is a three phase line which is bounded above and below by critical end points. A liquid-liquid critical line joins these two critical end points. There are several known configurations of the line joining the ends of the three phase line. In the example illustrated (fig. 1F) the liquid-liquid critical line has two branches with a region of complete liquid miscibility between them.

Most hydrocarbon + water systems studied to date exhibit type III phase behavior. Typical pressure-temperature-composition diagrams for type III behavior are illustrated in fig. 2A and 2B. The most common type of phase behavior found in hydrocarbon water mixtures corresponds to fig. 2A. The behavior shown in fig. 2B has not yet been observed in hydrocarbon + water systems. From fig. 1 and 2 it can be seen that the three phase line on the pressure-temperature projection is derived from three lines on the pressure-temperature-composition diagram representing, the composition of gas, liquid 1 and liquid 2. Phase Behavior





There are many sub-types of type III behavior. Consider the portion of the phase diagram in the region of the upper critical end point and the Consider the portion critical point of the pure component with the lower critical temperature. There are four possibilities. The three phase line could be at higher or lower pressures than the vapor pressure curve of the pure component. Each of these two cases could have the upper critical end point at a higher (or lower) temperature than the critical point. These four possibilities are illustrated in fig. 3. The position of the vapor pressure of the second component can be above or below that of the first component. In the case of hydrocarbon + water systems the two pure component vapor pressure curves sometimes cross on the pressure-temperature projection (e.g. benzene + water). Most hydrocarbons + water systems exhibit the behavior illustrated in fig. 3G. Consider fig. 3G, the three phase line is at higher pressures than the vapor pressure of the pure component (1). At a temperature, T_1 , the pressure-composition diagram is shown in fig. 3H. It can be seen that depending on the pressure and overall composition it is possible to have one, two, or three phases present. At high pressures we have a fluid-fluid equilibrium which if T_1 is sufficiently low, it is reasonable to refer to as a liquid-liquid equilibrium. Although a line parallel to the composition axis at pressures between the three phase line and the vapor-pressure of component (1) cuts the boundary lines in four places, only two phases can be in equilibrium. The two phases in equilibrium will depend on the overall composition. At temperature T_2 a different situation exists in that at pressures above the critical line it is possible to have two phases present (fig. 3I). At pressures below the critical point it is possible to have two phases coexisting out of a possible four phases. Which are the two coexist-ing phases dependings on the overall composition. At some compositions only one phase will be present.



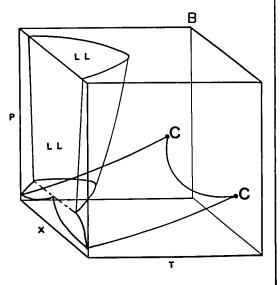


Fig. 4. Pressure, temperature, composition diagrams for two Type II systems. The three phase line is denoted -.-.-. The region in which two liquids coexist is denoted LL.

хх

Although most hydrocarbon + water systems studied to date exhibit type III phase behavior it is known that some hydrocarbons of greater molecular weight, such as biphenyl exhibit type II phase behavior⁶. Figures 4A and 4B illustrate the pressure-temperature-composition diagram for two type II systems. It appears that most, if not all, hydrocarbon + water systems which exhibit type II behavior have a minimum in temperature for the gas-liquid critical curve which corresponds to the behavior illustrated in fig. 4B.

Some hydrocarbon + water systems have been observed to exhibit the phenomenon referred to as gas-gas immiscibility $^{6'7}$. This phenomenon $^{5'8}$ occurs in type III phase behavior when the critical locus starting at the component with the highest critical temperature initially or eventually moves to high pressure at temperatures above the critical point of either component. If the critical locus always has a positive slope on the pressure-temperature projection the phenomenon is referred to as gas-gas immiscibility of the first kind (fig. 5A) whereas if the locus initially moves to lower temperatures, goes through a minimum and eventually moves to temperatures greater than the critical temperature of either component the mixture is said to exhibit gas-gas immiscibility of the second kind (fig. 5B). Gas-gas immiscibility of the second kind is exhibited by some hydrocarbon + water systems.

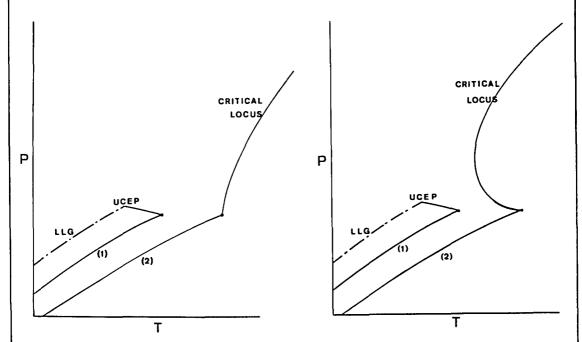


Fig. 5. Pressure, temperature projections for systems exhibiting gas-gas immiscibility. Figure 5A - immiscibility of the first kind. Figure 5B immiscibility of the second kind.

References.

- 1. Scott, R. L.; van Konynenburg, P. H.; Phil. Trans. Roy. Soc., London 1980, A298, 495.
- Hicks, C. P.; Young, C. L.; Chem. Rev. 1975, 75, 119.
 Gubbins, K. E.; Shing, K. S.; Streett, W. B.; J. Phys. Chem. 1983, 87, 4573.
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 Schneider, G. M.; in Chemical Thermodynamics Vol. 2, ed. M. L. McGlashan, A Specialist Periodical Report, The Chemical Society, London, 1978, Chap. 4.
- 6. Brollos, K.; Peter, K.; Schneider, G. M.; Ber. Bunsenges. Phys. Chem.
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 7. De Loos, Th. W.; Penders, W. G.; Lichtenthaler, R. N.; J. Chem. Thermodyn. 1982, 14, 83.
 8. Tsiklis, D. S.; Rott, L. A.; Russ. Chem. Rev. 1967, 36, 351.

COMPONENTS:	EVALUATOR:
<pre>(1) Styrene; C₈H₈; [100-42-5] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985

CRITICAL EVALUATION:

Quantitative solubility data for the styrene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1. Quantitative Solubility Studies of the Styrene (1) - Water (2) System

Reference	T/K	Solubility	Method
Lane (ref 1)	298-324	mutual	various ^a
Fordyce and Chapin (ref 2)	333	(l) in (2)	titration
Frilette and Hohenstein (ref 3)	298	(l) in (2)	unspecified
Andrews and Keefer (ref 4)	298	(l) in (2)	spectrophotometric
Banerjee <i>et al</i> . (ref 5)	298	(l) in (2)	HPLC

 α Chemical analysis and cloud point measurements for (1) in (2). Karl Fischer and cloud point measurements for (2) in (1).

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF STYRENE (1) IN WATER (2)

All the available data (ref 1-5) are listed in Table 2. At 298K the agreement among the independent measurements (ref 1,3-5) is reasonable but not sufficient to enable the average value to be Recommended.

At other temperatures, the value of Fordyce and Chapin (ref 2) at ~ 333K is very much higher than that of Lane (ref 1). Since the latter were obtained by two independent methods and, as already noted, are in fair agreement with other determinations at 298K, the datum of Fordyce and Chapin is rejected. In the absence of confirmatory studies the data at temperatures other than 298K should be regarded as very tentative.

(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) Styrene; C₈H₈; [100-42-5] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	July 1985.

CRITICAL EVALUATION: (continued)

TABLE 2. Tentative Values of the Solubilityof Styrene (1) in Water (2)

T/K	Solubility	values	
	Reported values ^a	"Best"'val	
	(g(l)/100g sln)	g(l)/100g sln	10 ⁵ x ₁
283	0.29* (ref l)	0.029	5.0
293	0.030* (ref 1)	0.030	5.2
298	0.033* (ref 1), 0.022 (ref 3), 0.030 (ref 4), 0.016 (ref 5)	0.025 ± 0.006^{b}	4.3
303	0.034* (ref 1)	0.034	5.9
313	0.040* (ref 1)	0.040	6.9
323	0.046* (ref 1)	0.046	8.0
333	0.053* (ref 1), 0.95 (ref 2) c	0.053	9.2

a Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the author's two data sets, followed by averaging.

b Average (± σ_n) of all data; σ_n has no statistical significance. c At T = 333.5K, value rejected: see text.

2. THE SOLUBILITY OF WATER (2) IN STYRENE (1)

The solubility of water in styrene has been reported in only one study (ref 1) and thus no Critical Evaluation is possible. The interested user is referred to the relevant data sheet for the experimental solubility values.

REFERENCES

1. Lane, W.H. Ind. Eng. Chem. Anal. Ed. 1946, 18, 295-6.

2. Fordyce, R.G.; Chapin, E.C. J. Am. Chem. Soc. 1947, 69, 581-3.

3. Frilette, V.J.; Hohenstein, W.P. J. Polym. Sci. <u>1948</u>, 3, 22-31.

4. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1950, 72, 5034-7.

 Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Env. Sci. Technol. <u>1980</u>, 14, 1227-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
	CALCUMAL MEASUREMENTS:	
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Lane, W.H.	
(2) Water; H ₂ O; [7732-18-5]	Ind. Eng. Chem. Anal. Ed. <u>1946</u> , 18, 295-6.	
	10, 200 00	
VARIABLES:	PREPARED BY:	
Temperature: 7-65°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
Solubility of	styrene in water	
t/°C g(1)100 ($\frac{10^5 x_1}{10^5 x_1}$ (compiler)	
(a) Formaldehyde - Sulfuric Acid	Reagent Method	
7 0.029	5.0	
24 0.033	5.7	
32 0.036	6.2	
40 0.040	6.9	
51 0.045	7.8	
(b) Cloud Point Method		
15 0.025	4.3	
25 0.031	5.3	
44 0.040	6.9	
49 0.045	7.8	
56 0.050	8.6	
65 0.058	10.0	
	ARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
(a) The solubility of (1) in (2)		
determined by means of the formal hyde-sulfuric acid reagent, ref (
The value shown for 7°C is the me		
of three determinations, and the value for 25°C is the mean of two		
determinations; all other data ar	e	
single determinations only. (b) The cloud point exhibited by	this	
system appeared to be very sharp, the samples passed from a state i		
which they were cloudy within 1°C	ESTIMATED ERROR:	
The cloud point data are averages from two to eight separate determ	of i- temp. (b) ± 0.5°C (from two to	
nations. Cloud points at 0.025 g		
100 g solution were very faint.	REFERENCES :	
	 Morris, H.E.; Stiles, R.B.; Lane, W.H. Ind. Eng. Chem. Anal. Ed. <u>1946</u>, 18, 294. 	

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Styrene; C ₈ H ₈ ; [100-4	2-5]	Lane, W.H.	
(2) Water; H ₂ O; [7732-18-		Ind. Eng. Chem. Anal. Ed. <u>1946</u> , 18, 295-6.	
VARIABLES:		PREPARED BY:	
Temperature: 6-51°C		A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:			
Solub	ility of wat	er in styrene	
t/°C	g(2)/100 g s	$10^3 x_2$ (compiler)	
(a) Karl Fischer Reagent	Method		
6	0.032	1.8	
24	0.066	3.8	
31	0.084	4.8	
40	0.101	5.8	
51	0.123	7.1	
(b) Cloud Point Method			
14	0.040	2.3	
27	0.060	3.5	
34	0.080	4.6	
40	0.100	5.7	
45	0.120	6.9	
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:	
 (a) A large sample of (1) ing a slight excess of (2) shaken at a given temperathen allowed to stand in bath at this temperature to ensure complete separathe two phases before wit sample of the rich phase tion of the water present Karl Fischer reagent. (b) Duplicate determination 	2) was ture and a water for 24 hr tion of thdrawal of for titra- with the	 (1) source not specified; fresh samples; used as received. (2) not specified. 	
cloud points agreeing wit except in the case of 0.1 100 g solution where the was within about 3°C. Cl at 0.040 (1)/100 g soluti very faint. No more deta reported.	hin 1°C, 20 g(1)/ agreement oud points on were	ESTIMATED ERROR: soly. (a) ± 1.5% (from two determi- nations) temp. (b) ± 1 to ± 3°C. REFERENCES:	

OMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Fordyce, R.G.; Chapin, E.C.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1947</u> , 69, 581-3.
VARIABLES:	PREPARED BY:
Dne temperature: 60.3°C	A. Maczynski
EXPERIMENTAL VALUES:	J <u></u>
The solubility of styrene in water at 100 g(2).	60.3 C was reported to be 0.96 g(l)/
The corresponding mass percent and mo compiler are 0.95 g(l)/l00 g sln and	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	SOURCE AND PURITY OF MATERIALS: (1) Dow Chemical Co, N-100; redistilled.
METHOD/APPARATUS/PROCEDURE: Into two stoppered 50 mL Erlenmeyer Elasks were weighed two 25.000 g por-	SOURCE AND PURITY OF MATERIALS; (1) Dow Chemical Co, N-100; redistilled.
METHOD/APPARATUS/PROCEDURE: Into two stoppered 50 mL Erlenmeyer flasks were weighed two 25.000 g por- tions of (2). The flasks were placed in a water-bath regulated to $60.3 \pm$ 0.02°C. Component (1) was added a drop at a time to the water samples by means of a calibrated micro-pipet and the flasks agitated after each addition. The saturation point was taken at the first appearance of the	SOURCE AND PURITY OF MATERIALS; (1) Dow Chemical Co, N-100; redistilled.
METHOD/APPARATUS/PROCEDURE: Into two stoppered 50 mL Erlenmeyer flasks were weighed two 25.000 g por- tions of (2). The flasks were placed in a water-bath regulated to 60.3 ± 0.02°C. Component (1) was added a drop at a time to the water samples by means of a calibrated micro-pipet and the flasks agitated after each addition. The saturation point was taken at the first appearance of the curbidity and the amount of (1) was calculated from the number of drops	<pre>SOURCE AND PURITY OF MATERIALS: (1) Dow Chemical Co, N-100; redistilled. (2) Not specified. ESTIMATED ERROR: temp. ±0.02°C</pre>
METHOD/APPARATUS/PROCEDURE: Into two stoppered 50 mL Erlenmeyer flasks were weighed two 25.000 g por- tions of (2). The flasks were placed in a water-bath regulated to 60.3 ± 0.02°C. Component (1) was added a drop at a time to the water samples by means of a calibrated micro-pipet and the flasks agitated after each addition. The saturation point was taken at the first appearance of the curbidity and the amount of (1) was calculated from the number of drops	<pre>SOURCE AND PURITY OF MATERIALS: (1) Dow Chemical Co, N-100; redistilled. (2) Not specified. ESTIMATED ERROR: temp. ±0.02°C soly. ±0.05 g(1)/100 g sln</pre>
METHOD/APPARATUS/PROCEDURE: Into two stoppered 50 mL Erlenmeyer flasks were weighed two 25.000 g por- tions of (2). The flasks were placed in a water-bath regulated to 60.3 ± 0.02°C. Component (1) was added a drop at a time to the water samples by means of a calibrated micro-pipet and the flasks agitated after each addition. The saturation point was taken at the first appearance of the curbidity and the amount of (1) was calculated from the number of drops	<pre>SOURCE AND PURITY OF MATERIALS: (1) Dow Chemical Co, N-100; redistilled. (2) Not specified. ESTIMATED ERROR: temp. ±0.02°C</pre>
METHOD/APPARATUS/PROCEDURE: Into two stoppered 50 mL Erlenmeyer flasks were weighed two 25.000 g por- tions of (2). The flasks were placed in a water-bath regulated to 60.3 ± 0.02°C. Component (1) was added a drop at a time to the water samples by means of a calibrated micro-pipet and the flasks agitated after each addition. The saturation point was taken at the first appearance of the curbidity and the amount of (1) was calculated from the number of drops	<pre>SOURCE AND PURITY OF MATERIALS: (1) Dow Chemical Co, N-100; redistilled. (2) Not specified. ESTIMATED ERROR: temp. ±0.02°C soly. ±0.05 g(1)/100 g sln</pre>

	1

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Frilette, V.J.; Hohenstein, W.P.	
(2) Water; H ₂ O; [7732-18-5]	J. Polym. Sci. <u>1948</u> , 3, 22-31.	
VARIABLES:	DEDADED NY.	
	PREPARED BY:	
One temperature: 25°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
The solubility of styrene in water at 25°C was reported to be 0.022 g(1)/100 g sln.		
The corresponding mole fraction, x_1 , compilers is 3.8 x 10 ⁻⁵ .	value calculated by the	
	······	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The saturated solutions of (1) in (2) were prepared in two different	(1) not specified.	
ways. In the first method, conju- gated solutions were prepared by	(2) distilled.	
shaking together excess (1) with (2) and allowing the layers to		
separate; the aqueous layer was then analyzed for (1). To avoid		
the possibility of contaminating the aqueous phase by small suspended		
droplets a second method was uti- lized; a cellophane sack, filled		
with (2) was completely submerged in a beaker containing (2); a layer	ESTIMATED ERROR:	
of (1) was then floated on top of (2) in the beaker. After 48 hr at	Not specified.	
25°C, the sack was retrieved and the contents carefully removed and analyzed.	REFERENCES:	
The method of analysis was not described.		

	7
	ORIGINAL MEASUREMENTS:
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of styrene in water at	25° C was reported to be 0.030 g(1)/
100 g sln.	25 0 was reperced to be 0.050 g(r//
The corresponding mole fraction, x_1 , c	calculated by the compilers is
5.19 x 10^{-5} .	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant tem-	 Eastman Kodak Co. white label; distilled shortly before use;
perature bath at 25°C. A sample (5-20 mL) of the aqueous phase was	l wt % of hydroquinone added as stabilizer before distilla-
withdrawn and extracted with a mea- sured volume of hexane (10-50 mL) by	tion; b.p. 76 C (78 mm Hg).
shaking in a glass-stoppered Erlen-	(2) Not specified.
meyer flask. Next, the absorbance of the hexane phase was measured against	
a hexane blank on the Beckman spec- trophotometer.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Styrene; C ₈ H ₈ ; [100-42-5] (2) Water; H ₂ O; [7732-18-5]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Environ. Sci. Technol. <u>1980</u> , 14, 1227-9.
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of styrene in water wa sln. Assuming a solution density of per cent and mole fraction (x ₁) solub are 0.0160 g(1)/100 g sln and 2.77 x	1.00 kg/L the corresponding mass bilities, calculated by the compiler,
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Experiments were performed in sealed stainless steel centrifuge tubes. An excess of styrene was added to a tube containing distilled water, and the tube was sealed and allowed to equi- librate at $25 \pm 0.2^{\circ}$ C with constant or intermittent shaking. Equilibra- tion was generally complete within 1 week. The mixture was then centri- fuged at 10,000 rpm for 60 min in a head preequilibrated to $25 \pm 0.3^{\circ}$ C, following which aliquots of the solu- tion were removed for analysis by high-performance liquid chromato- graphy using a Waters M6000A instru- ment fitted with a C18 Bondapak column. The mobile phase was a mix- ture of methanol/water or aceto- nitrile/water. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.	(2) Distilled.
	L

COMPONENTS:	EVALUATOR:
<pre>(1) o-Xylene; C₈H₁₀; [95-47-6] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	July 1985.

CRITICAL EVALUATION:

Quantitative solubility data for the o-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies ofthe o-Xylene (1) - Water (2) System

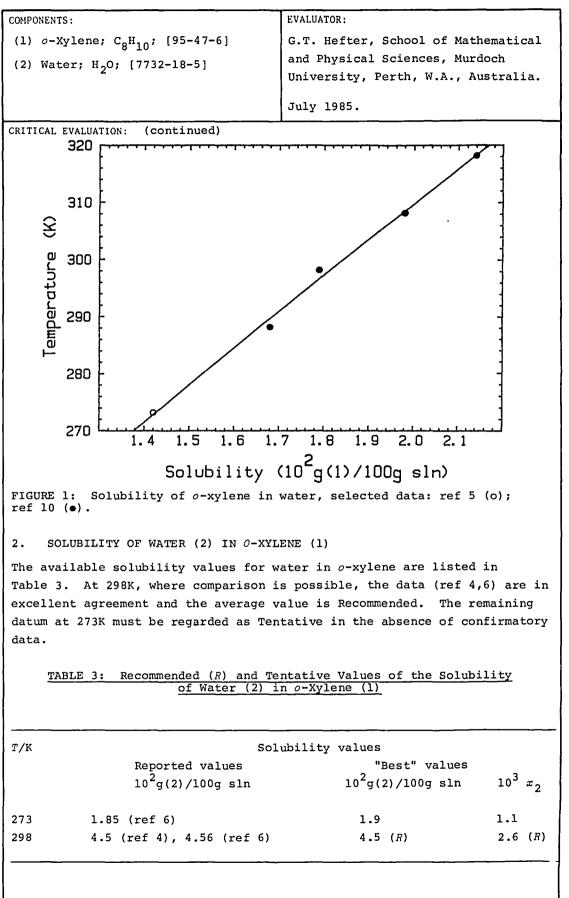
Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Guseva and Parnov (ref 2)	385-524	(1) in (2)	unspecified
McAuliffe (ref 3)	298	(l) in (2)	GLC
Hoegfeldt and Bolander (ref 4)	298	(2) in (1)	Karl Fischer
Polak and Lu (ref 6)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 7)	298	(1) in (2)	GLC
Price (ref 8)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 9)	298	(1) in (2)	GLC
Sanemasa $et \ al.$ (ref 10)	299-318	(1) in (2)	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Alwani and Schneider (ref 5) have also reported data on a critical locus at high temperatures and pressures. For convenience further discussion of this system will be given in two parts.

1. SOLUBILITY OF O-XYLENE (1) IN WATER (2)

The high temperature, high pressure data of Guseva and Parnov (ref 2) and Alwani and Schneider (ref 5) have been obtained under quite different conditions and thus no Critical Evaluation of their data is possible. However, it may be noted that the data of Guseva and Parnov are frequently unreliable. The interested user is referred to the relevant Data Sheets for experimental values.

At atmospheric pressure all the available data are listed in Table 2 except for the value of Krzyzanowska and Szeliga (ref 9) which does not appear to be independent of that of Price (ref 8) and has therefore been excluded from consideration.



(continued next page)

COMPONENTS: (1) <i>o</i> -Xylene; C ₈ H ₁₀ ; [95-47-6] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	July 1985

CRITICAL EVALUATION: (continued)

At 298K, the data of McAuliffe (ref 3), Sutton and Calder (ref 7), Price (ref 8) and Sanemasa *et al.* (ref 10) are in excellent agreement and their average is Recommended. The values of Andrews and Keefer (ref 1) and Polak and Lu (ref 6) are markedly higher ($>3\sigma_n$) and are rejected.

At other temperatures only the data of Sanemasa $et \ all$. (ref 10) are available except for the 273K datum of Polak and Ly (ref 6). These data are therefore regarded as Tentative.

Selected data are plotted in Figure 1.

TABLE 2: Recommended (R) and Tentative Solubility Values ofo-Xylene (1) in Water (2)

<i>т/</i> к	Solubilit Reported values 10 ² g(1)/100g sln	ty values "Best" values 10 ² g(1)/100g sln	
273	1.42 (ref 5)	1.4	2.4
288	1.68 (ref 10)	1.7	2.9
298	1.75 (ref 3), 1.705 (ref 7), 1.67 (ref 8), 1.79 (ref 10)	1.73 ± 0.05 (R)	2.93 (R)
308	1.98 (ref 10)	2.0	3.4
318	2.14 (ref 10)	2.1	3.6

a Obtained by averaging where appropriate; $\sigma_{\rm n}$ has no statistical significance.

(continued next page)

COMPONENTS: EVALUATOR: (1) o-Xylene; C₈H₁₀; [95-47-6] G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. July 1985 (continued) CRITICAL EVALUATION: REFERENCES 1. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1949, 71, 3644-7. Guseva, A.N.; Parnov, E.I. Vestn. Mosk. Univ. Khim. 1963, 18, 76-9. 2. 3. McAuliffe, C. Nature 1963, 200, 1092-3; J. Phys. Chem. 1966, 70, 1267-72. 4. Hoegfeldt, E.; Bolander, B. Ark. Kemi 1964, 21, 161-86. Alwani, Z.; Schneider, G.M. Ber. Bunsenges. 1969, 73, 294-301. 5. Polak, J.; Lu, B. C-Y. Can. J. Chem. 1973, 51, 4018-23. 6. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2. 7. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44; see also Ph.D. Dissertation, 1973, Univ. California, Riverside, CA, U.S.A., 8. quoted in ref 10. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7. 9. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62. 10. ACKNOWLEDGEMENT The Evaluator thanks Dr Brian Clare for the graphics.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of o-Xylene in water at 0.0204 g(l)/100 g sln.	t 25°C was reported to be
The corresponding mole fraction, x_1 , x_3 .46 x 10^{-5} .	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant tem-	(1) Eastman Kodak Co. best grade; fractionally distilled; b.p.
perature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a	range 144.3-144.5°C.
measured volume of hexane (10-50 mL) by shaking in a glass-stoppered	(2) Not specified.
Erlenmeyer flask. Next, the absorb- ance of the hexane phase was meas-	
ured against a hexane blank on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:
	3

			OPTOTWAL WEACHDENENDER	
COMPONENTS: (1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]		95-47-61	ORIGINAL MEASUREMENTS: Guseva, A.N.; Parnov, E.I.	
			Vestn. Mosk. Univ. Khim. <u>1963</u> ,	18
(2) Water; H ₂	0; [7/32	10-71	76-9.	10,
	······			
VARIABLES:			PREPARED BY:	
Temperature:	139-251°(2	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALU	ES:	······································		
	Sol	lubility of o-	xylene in water	
	t/°C	g(1)/100 g	sln $10^4 x_1$ (compiler)	
	139 162	0.047 0.093	0.80 1.58	
	207 251	0.407 0.960	6.93 16.42	
		AUXILIARY	INFORMATION	
METHOD/APPARATUS/			SOURCE AND PURITY OF MATERIALS;	
The measureme sealed glass	tubes. No	details	(1) source not specified; n _D ²⁰ 1.5054.	
were reported	in the pa	per.	ⁿ D ^{1.3034} .	
			(2) doubly distilled.	
			ESTIMATED ERROR:	
			not specified.	
			1	
			REFERENCES:	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) <u>1963</u> , 200, 1092-3.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of o-Xylene in water at	z 25°C was reported to be
0.0175 g(1)/100 g sln.	
The corresponding mole fraction, x_1 , or 2.97×10^{-5} .	calculated by the compilers is
2.97 x 10 .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solution of (1) in (2) was prepared by either shaking vigor-	(1) Phillips Petroleum Co.; 99+%; used as received.
ously on a reciprocal shaker or stir-	
ring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample	(2) Distilled.
of the hydrocarbon-saturated water was injected directly into a gas	
liquid chromatograph.	
	ESTIMATED ERROR:
	Temp. ±1.5°C
	Soly. 0.0008 (std. dev. of mean)
	REFERENCES :
``````````````````````````````````````	

ORIGINAL MEASUREMENTS: COMPONENTS: o-Xylene; C₈H₁₀; [95-47-6] Hoegfeldt, E.; Bolander, B. (1) Water; H₂O; [7732-18-5] Ark. Kemi, 1964, 21, 161-86. (2) VARIABLES: PREPARED BY: One temperature: 25°C A. Maczynski and Z. Maczynska EXPERIMENTAL VALUES: The solubility of water in o-Xylene was reported to be 0.022 mol(2) L sln. The corresponding mass percent and mol fraction,  $x_2$ , calculated by the compilers are 0.045 g(2)/100 g sln and 0.0026. The assumption that 1.00 L sln = 876 g sln was used in the calculation. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The water determination was carried (1) Fluka; 0.7% of (m-p) xylene, out according to Johansson's modifi-cation of the Karl Fischer titration 0.07% of ethylbenzene; purity 99.0%; used as received. in ref 1, 2. ESTIMATED ERROR: Temp. ±0.3 C Soly. ±0,002 mol(2) L⁻¹ sln (type of error not specified) **REFERENCES:** 1. Hardy, C.J.; Greenfield, B.F.; Scargill, D. J. Chem. Soc. 1961, 90. 2. Johansson, A. Sv. Papperstidn. 1947, 11B, 124.

				1
COMPONENTS:			ORIGINAL MEASUREME	NTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]		Polak, J.; Lu, B.CY.		
(2) Water; H ₂ O; [7732-18-5]		Can. J. Chem.	<u>1973</u> , <i>51</i> , 4018-23.	
VARIABLES:		<u> </u>	PREPARED BY:	
Temperature: 0-25°C		A. Maczynski and Z. Maczynska		
EXPERIMENTAL	VALUES:			
	Solubility	of o-;	ylene in water	
t/°C	mg(l)/kg(2)	g (]	)/100 g sln (compiler)	10 ⁵ x ₁ (compiler)
0(a)	142(c)		0.0142	2.41
25(b)	213(c)		0.0213	3.61
	Solubility	of wat	er in o-xylene	
t∕°C	mg(2)/kg(1)	g (2	2)/100 g sln (compiler)	$10^{3}x_{2}$ (compiler)
 0 (a)	185 (d)		0.0185	1.09
25 (b)	456 (e)		0.0456	2.68
	AL	JXILIARY	INFORMATION	
METHOD/APPARA	TUS/PROCEDURE:		SOURCE AND PURITY	OF MATERIALS:
with (2) w Hypo-vial teflon coa placed in water bath magnetical the bath w	ely 50 mL of (1) tog vere placed in a 125 m which was closed wit ated rubber septum an a constant-temperatu a. The system was st ly for 24 hr and lef for 3 days or was kep without stirring for ore samples were take	nL h a d re irred t in t in 7	reagent; s	ganics, pure grade haken three times lled water.
for analysis. The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.		ESTIMATED ERROR: temp. (a) ± 0.02°C, (b) ± 0.01°C soly. (c) ± 1.7%, (d) ± 4.7%, (e) ± 3.1% (from two or three determinations) REFERENCES:		

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of o-xylene in water a	at 25°C was reported to be
170.5 mg(l)/kg(2). The corresponding	g mass percent and mole fraction,
$x_1$ , calculated by the compilers are (	).01705 g(1)/100 g sln and
$2.892 \times 10^{-5}$ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The concentration of (1) in (2) was determined by gas chroma-	SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemical Co. or Matheson Coleman and Bell
tography.	99+%.
	(2) distilled.
	ESTIMATED ERROR:
	temp. $\pm 0.1^{\circ}$ C soly. 2.5 mg(1)/kg(2)
	(the standard deviation of the mean for six replicates)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [97-47-6]	Krzyzanowska, T.; Szeliga, J.
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	I
EATENINE VALUES.	
The solubility of o-xylene in water	at 25°C was reported
to be 167.0 mg(1)/kg(2).	
The corresponding mass percent and m	ole fraction, $x_1$ , calculated
by compiler are 0.0167 g(l)/100 g sl	n and 2.83 x $10^{-5}$ .
	a star at the budrogerbon water
Editor's Note: Based on the results systems, uncertainity exists about w	for this and other hydrocarbon-water bether the datum compiled here is
independent of that of Price for the	same system (see previous page).
Independent of end of a	-
·······	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways.	(1) not specified.
First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted	(2) not specified.
at 25°C. Second, the mixture of (1)	
and (2) as above was thermostated at 70°C and then cooled to 25°C. The	e
time required to obtain equilibrium was three weeks. The solubility of	
(1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	
ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame	ESTIMATED ERROR:
ionization detector was used. Sat-	
urated solutions of heptane in (2) were used as standard solutions.	soly. 4.2 mg(1)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES:
Î.	}

OMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) <i>o</i> -Xylene; C ₈ H ₁₀ ; [97-47-6] (2) Water; H ₂ O; [7732-18-5]		Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 1982, 55, 1054-62		
ARIABLES:		PREPARED BY:		
Temperature: 15-45°C		G.T. Hefter	G.T. Hefter	
XPERIMENTAL VAL	JES:	" <b>L</b> ,	. <u></u>	
	The solubility of	o-xylene in water		
<i>t</i> /°C	10 ³ mol(1)/dm ³ sln	g(1)/100 g sln (compiler) ^a	$10^5 x_1$ (compiler) ^a	
15	$1.58 \pm 0.11$	0.0168	2.85	
25	$1.68 \pm 0.06$	0.0179	3.04	
35	$1.85 \pm 0.02$	0.0198	3.35	
45	$2.00 \pm 0.02$	0.0214	3.64	
	solution densities to be temperature (ref 1).	the same as those of	pure water at	
		the same as those of	pure water at	
	temperature (ref 1).	the same as those of	pure water at	
the same f	temperature (ref 1). AUXILIARY			
The same of THOD/APPARATUS The apparatus carlier design lescribed in c .00-200 cm ³ of .iquid (1) were out connected .ished a recin vas used to va .co transport to .co transport to	AUXILIARY /PROCEDURE: is similar to an h (ref 2) and is letail in the paper. f (2) and 10-20 cm ³ of ce placed in separate thermostatted flasks. equilibrium was estab- culating stream of air aporize liquid (1) and the vapor to the flask . Five 10 cm ³ aliquots	INFORMATION SOURCE AND PURITY OF MAT (1) Analytical read Pure Chemical : purity 98.0%, u further purific (2) Redistilled; no given.	ERIALS: gent grade (Wako Ind. Ltd.), state ised without	
the same to the same to the apparatus arlier design escribed in co 00-200 cm ³ of iquid (1) were out connected fter thermal ished a recin vas used to va co transport to ontaining (2) vere withdrawn	AUXILIARY /PROCEDURE: is similar to an h (ref 2) and is letail in the paper. f (2) and 10-20 cm ³ of ce placed in separate thermostatted flasks. equilibrium was estab- culating stream of air aporize liquid (1) and the vapor to the flask 5. Five 10 cm ³ aliquots h into separatory	INFORMATION SOURCE AND PURITY OF MAT (1) Analytical read Pure Chemical : purity 98.0%, u further purific (2) Redistilled; no given.	ERIALS: gent grade (Wako Ind. Ltd.), state ised without cation.	
the same to ETHOD/APPARATUS The apparatus arlier design escribed in co 00-200 cm ³ of iquid (1) were out connected fter thermal ished a recin tas used to vare o transport to ontaining (2) were withdrawn unnels. The 2) was then co nto chlorofor pectrophotome	AUXILIARY /PROCEDURE: is similar to an h (ref 2) and is letail in the paper. f (2) and 10-20 cm ³ of ce placed in separate thermostatted flasks. equilibrium was estab- culating stream of air aporize liquid (1) and the vapor to the flask . Five 10 cm ³ aliquots	<pre>INFORMATION SOURCE AND PURITY OF MAT (1) Analytical read Pure Chemical : purity 98.0%, u further purific (2) Redistilled; no given. ESTIMATED ERROR: soly. see table, typ provision</pre>	ERIALS: gent grade (Wako Ind. Ltd.), state ised without cation. o further detail	
the same of ETHOD/APPARATUS The apparatus arlier design escribed in c 00-200 cm ³ of iquid (1) wer out connected fter thermal ished a recin vas used to va o transport of ontaining (2) were withdrawn unnels. The 2) was then con nto chlorofon pectrophotome	AUXILIARY AUXILIARY /PROCEDURE: is similar to an h (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of ce placed in separate thermostatted flasks. equilibrium was estab- culating stream of air aporize liquid (1) and the vapor to the flask . Five 10 cm ³ aliquots h into separatory concentration of (1) in determined by extraction cm followed by UV- etry. Standards for the	<ul> <li>INFORMATION</li> <li>SOURCE AND PURITY OF MAT         <ol> <li>Analytical read Pure Chemical : purity 98.0%, u further purific</li> <li>Redistilled; no given.</li> </ol> </li> <li>ESTIMATED ERROR: soly. see table, typ specified.</li> </ul>	ERIALS: gent grade (Wako Ind. Ltd.), state ised without cation. o further details	
the same to the same to the same to the apparatus the apparatu	AUXILIARY AUXILIARY /PROCEDURE: is similar to an h (ref 2) and is letail in the paper. f (2) and 10-20 cm ³ of ce placed in separate thermostatted flasks. equilibrium was estab- culating stream of air aporize liquid (1) and the vapor to the flask b. Five 10 cm ³ aliquots h into separatory concentration of (1) in letermined by extraction cm followed by UV- etry. Standards for the etry were prepared by	<pre>INFORMATION SOURCE AND PURITY OF MAT (1) Analytical read Pure Chemical : purity 98.0%, u further purific (2) Redistilled; nd given. ESTIMATED ERROR: soly. see table, typ specified. temp. ± 0.1°C.</pre>	ERIALS: gent grade (Wako Ind. Ltd.), state used without cation. o further details pe of error not	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	Sutton, C.; Calder, J.A.
(2) Artificial seawater (ref 1)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES: One temperature: 25.0°C	PREPARED BY:
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of o-xylene in artifi	cial seawater is reported to be
 129.6 mg(1)/kg sln. The correspondi	
$x_1$ calculated by the compiler are 0.	
assuming the artificial seawater com	position of ref 1.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A test tube containing (1) was placed in a flask containing (2)	(1) from either Aldrich Chemical Co. or Matheson Coleman and
thus allowing for equilibration through the vapor phase. The	Bell, 99+% pure.
saturated solution was extracted	(2) made from doubly distilled
with hexane and analyzed by gas chromatography.	water and salts 99+% pure.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 1.8 (std. dev.)
	REFERENCES :
	<ol> <li>Lyman, J.; Fleming, R.H.; J. Mar. Res. 1940, 3, 135.</li> </ol>
	, ,

COMPONENTS:	EVALUATOR:
(2) Water; $H_00$ ; $[7732-18-5]$	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986

CRITICAL EVALUATION:

Quantitative solubility data for the m-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies ofthe m-Xylene (1) - Water (2) System

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 2)	274-313	(1) in (2)	spectrophotometric
Pryor and Jentoft (ref 3)	344-544	(1) in (2)	synthetic
Guseva and Parnov (ref 4)	400-512	(1) in (2)	${\tt unspecified}^a$
Hoegfeldt and Bolander (ref 5)	298	(2) in (1)	Karl Fischer
Englin $et \ al.$ (ref 6)	283-303	(2) in (1)	analytical
Polak and Lu (ref 7)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 8)	298	(1) in (2)	GLC
Chernoglazova and Simulin (ref 9)	293-343	mutual	synthetic, GLC
Price (ref 10)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 11)	298	(l) in (2)	GLC
Sanemasa <i>et al</i> . (ref 12)	288-318	(1) in (2)	spectrophotometric

a The synthetic method was probably used.

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into three parts.

#### SOLUBILITY OF M-XYLENE (1) IN WATER (2)

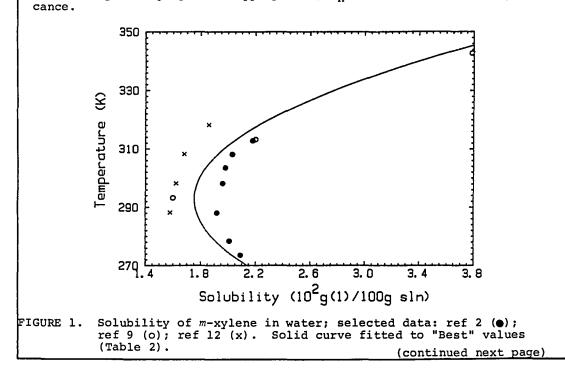
All the available data for the solubility of *m*-xylene in water at low temperatures ( $T \leq 343$ K) are summarized in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 11) which does not appear to be independent of that of Price (ref 10) and has therefore been excluded from consideration.

The data are in general in reasonable agreement although with a few exceptions the agreement is insufficient for the average values to be Recommended. Selected data from Table 2 are plotted in Figure 1.

COMPONENTS:	EVALUATOR:
	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986

TABLE 2: Recommended (R) and Tentative Values of the Solubility of m-Xylene (1) in Water (2)

<i>т/</i> к	Solubili	Solubility values			
	Reported values ^a	"Best" values $(\pm \sigma_n)^b$ 10 ² g(1)/100g sln 10 ⁵ $x_1$			
	10 ² g(1)/100g sln	10 ² g(1)/100g sln	$10^{5} x_{1}$		
273	2.10* (ref 2), 1.96 (ref 7)	$2.03 \pm 0.07 (R)$	3.44 (R)		
283	1.97* (ref 2)	2.0	3.4		
293	1.95* (ref 2), 1.6 (ref 9) 1.60* (ref 12)	1.7 ± 0.2	2.9		
298	1.73 (ref 1), 1.96 (ref 2), 1.62 (ref 7), 1.46 (ref 8), 1.7* (ref 9), 1.34 (ref 10), 1.62 (ref 12)	1.6 ± 0.2	2.7		
303	l.98* (ref 2), l.8* (ref 9), l.65* (ref 12)	1.8 ± 0.1	3.1		
313	2.19* (ref 2), 2.2 (ref 9)	2.20 (R)	3.73 (R)		
323	2.6* (ref 9), 2.0* (ref 12)	2.3 ± 0.3	3.9		
333	3.2* (ref 9)	3.2	5.4		
343	3.5* (ref 3)	3.5	5.9		
graph	es marked with an asterisk (*) have nical interpolation of the authors' ined by averaging where appropriate	original data.			



COMPONENTS :	EVALUATOR:
<pre>(1) m-Xylene; C₈H₁₀; [108-38-3] (2) Water; H₂O [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986.

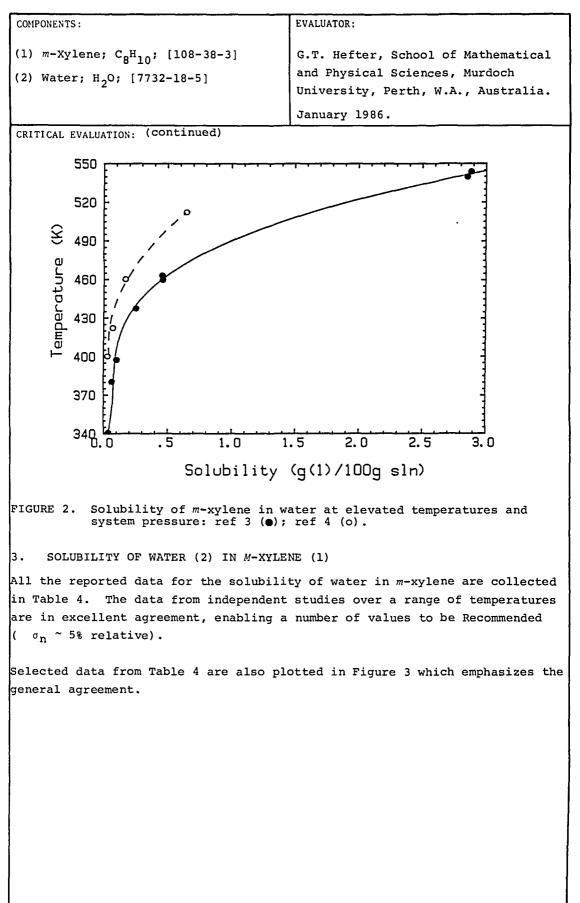
Table 3 summarizes thermodynamic functions calculated by application of the van't Hoff equation to the solubility data obtained over various temperature ranges. At low temperatures (T < 343K) the values of  $\Delta H_{sln}$  and  $\Delta C_{p,sln}$  from the data of Bohon and Claussen (ref 2) and Sanemasa *et al.* (ref 12) are in good agreement (Table 3) and are close to calorimetric values reported for similar systems (*e.g.* benzene in water, ref 13). However, the  $\Delta H_{sln}$  derived from the data of Chernoglazova and Simulin (ref 9) is much too positive.

## TABLE 3: Thermoydnamic Function for the Dissolution of m-Xylene in Water Derived from Solubility Data

Reference	^{ΔH} sln	ΔC _{p,sln} J K ^{-l} mol-l
	kJ mol ⁻¹	J K ⁻¹ mol-1
Bohon and Claussen (ref 2)	2.8	386
Pryor and Jentoft (ref 3)	8.6	200
Guseva and Parnov (ref 4)	36.7	55
Chernoglazova and Simulin (ref 9)	11.4	167
Sanemasa (ref 12)	2.6	317
"Best" values (Table 2)	2.9	516

2. SOLUBILITY OF M-XYLENE (1) IN WATER (2) AT ELEVATED TEMPERATURES

Solubility data for *m*-xylene in water at elevated temperatures (*ca.* 340-550K) and system pressure in sealed tubes have been reported by Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 14). The results are plotted in Figure 2 and are clearly in poor agreement. In the absence of comfirmatory studies it is difficult to know which values are more reasonable. However, it may be noted that the thermodynamic functions derived from the data of Pryor and Jentoft are more reasonable than those obtained from Guseva and Parnov's work (Table 3). The interested user is referred to the relevant Data Sheets for the experimental values.

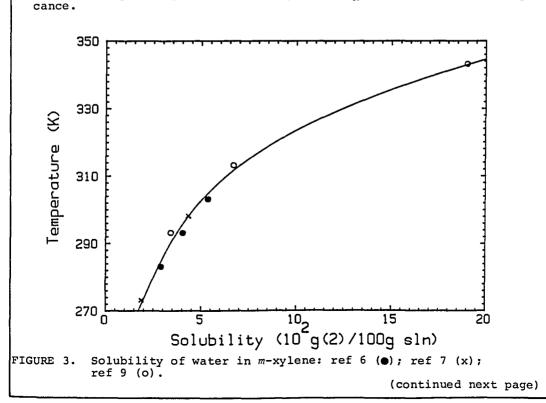


COMPONENTS:	EVALUATOR:
<pre>(1) m-Xylene; C₈H₁₀; [108-38-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986.
CRITICAL EVALUATION: (continued)	

# TABLE 4: Recommended (R) and Tentative Values of the Solubility of Water (2) in m-Xylene (1)

T/K	Solubility values						
	Reported values ^a	"Best" values	$(\pm \sigma_n)^b$				
	10 ² g(2)/100g sln	10 ² g(2)/100g sln	$10^{3}x_{2}$				
273	1.88 (ref 7)	1.9	1.1				
283	2.89 (ref 6), 2.8* (ref 7)	$2.9 \pm 0.1 (R)$	1.7(R)				
293	4.02 (ref 6), 3.7* (ref 7), 3.4 (ref 9)	3.7 ± 0.3 (R)	<b>2.2</b> ( <i>R</i> )				
298	4.4 (ref 5), 4.7* (ref 6), 4.32 (ref 7), 4.0 (ref 9)	4.4 ± 0.3 (R)	<b>2.6</b> ( <i>R</i> )				
303	5.36 (ref 6), 4.8 (ref 9)	5.1 ± 0.3 (R)	3.0(R)				
313	6.7 (ref 9)	6.7	6.7				
323	10* (ref 9)	10	5.9				
333	14* (ref 9)	14	8.3				
343	19* (ref 9)	19	11				

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data. b Calculated by averaging where appropriate;  $\sigma_n$  has no statistical signifi-



COMPONENTS:	EVALUATOR:
<pre>(1) m-Xylene; C₈H₁₀; [108-38-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

Application of the van't Hoff equation to the data of Englin *et al*. (ref 6) and Chernoglazova and Simulin (ref 9) gives values for  $\Delta H_{sln}$  of 21.3 and 24.9 kJ mol⁻¹ and for  $\Delta C_{p,sln}$  of -152 and 208 J K⁻¹ mol⁻¹ respectively. Comparison with related systems (*e.g.* water in benzene) suggests the data of Chernoglazova and Simulin (ref 9) may be more reliable.

REFERENCES

1.	Andrews,	L.J.;	Keefer,	R.M.	J.	Am.	Chem.	Soc.	<u>1949</u> ,	71,	3644-7	7.
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- 2. Bohon, R.L.; Claussen, W.F. J. Am. Chem. Soc. <u>1951</u>, 73 1571-8.
- 3. Pryor, W.A.; Jentoft, R.E. J. Chem. Eng. Data <u>1961</u>, 6, 36-7.
- 4. Guseva, A.N.; Parnov, E.T. Vestn. Mosk. Univ. Khim. <u>1963</u>, 18, 76-9.
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- 8. Sutton, C.; Calder, J.A. J. Chem. Eng. Data <u>1975</u>, 20, 320-2.
- Chernoglazova, F.S.; Simulin, Yu.N. Zh. Fiz. Khim. <u>1976</u>, 50, 809; Deposited doc. 1976, VINITI 3528-75.
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- 11. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) <u>1978</u>, 34, 413-7.
- 12. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62.
- 13. Gill, S.J.; Nichols, N.F.; Wadso, I. J. Chem. Thermodyn. <u>1976</u>, 8, 445-52.

#### ACKNOWLEDGEMENT

The evaluator thanks Dr Brian Clare for the regression analyses and graphics.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
	<u></u> , -1,
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of m-Xylene in water a	$t^{25}$ °C was reported to be
010173 g(1)/100 g sln.	
The corresponding mole fraction, $x_1$ , 2.93 x 10 ⁻⁵ .	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant tem-	(1) Eastman Kodak Co. best grade; fractionally distilled;
perature bath at 25°C. A sample (5-20 mL) of the aqueous phase was	b.p. 139.5°C.
withdrawn and extracted with a mea- sured volume of hexane (10-50 mL)	(2) Not specified.
by shaking in a glass-stoppered	
Erlenmeyer flask. Next, the absorb- ance of the hexane phase was mea-	
sured against a hexane blank on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	1

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Bohon, R.L.; Claussen, W.F.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1951</u> , 73, 1571-8.
VARIABLES:	PREPARED BY:
Temperature: 0.4-39.6°C	G.T. Hefter
EXPERIMENTAL VALUES:	
_	-xylene in water Dog sln ^a 10 ⁵ x1
	$\begin{array}{ccc} \log \ \sin^a & 10^3 x_1 \\ \text{piler}) & (\text{compiler}) \\ \hline \end{array}$
0.4 0.0	3.54
	3.41
	0192 3.25 0196 3.33
	$3.33^{b}$
	3.33
	3.36
	0203 3.44 0218 3.69
"extinction coefficients" (absorptive densities. This gave a solubility of converted to g(1)/100g sln by assumin ^b Given in the original paper as 0.1969	f g(1)/L sln which was then ng a solution density of 1.00 kg/L.
densities. This gave a solubility of converted to g(1)/100g sln by assumin	f g(1)/L sln which was then ng a solution density of 1.00 kg/L.
densities. This gave a solubility of converted to g(1)/100g sln by assumin ^b Given in the original paper as 0.1969	f g(1)/L sln which was then ng a solution density of 1.00 kg/L.
densities. This gave a solubility of converted to g(l)/100g sln by assumin ^b Given in the original paper as 0.1969	f g(1)/L sln which was then ng a solution density of 1.00 kg/L. g(1)/L sln.
densities. This gave a solubility of converted to g(l)/100g sln by assumin ^b Given in the original paper as 0.1969 AUXILIARY	<pre>f g(1)/L sln which was then ng a solution density of 1.00 kg/L. g(1)/L sln. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Oronite Chemical Co. was sulphonated, hydrolysed, steam distilled, washed, dried by passing through silica gel and finally distilled. Purity was</pre>
densities. This gave a solubility of converted to g(1)/100g sln by assumine ^b Given in the original paper as 0.1969 AUXILIARY METHOD/APPARATUS/PROCEDURE: A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls	<pre>f g(1)/L sln which was then ng a solution density of 1.00 kg/L. g(1)/L sln. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Oronite Chemical Co. was     sulphonated, hydrolysed, steam     distilled, washed, dried by     passing through silica gel and     finally distilled. Purity was     judged by refractometry (no     value given). (2) Air-free conductivity water (no     details given). ESTIMATED ERROR: Temp. ± 0.02°C Soly. ± 0.5% relative</pre>

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Pryor, W.A.; Jentoft, R.E.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1961</u> , 6, 36-7.
VARIABLES:	PREPARED BY:
Temperature: 67.7-270.6°C	A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

## Solubility of m-xylene in water

Cloud point appears	t/°C Cloud point disappears	Midpoint	10 ³ <i>x</i> ₁	g(l)/100 g sln (compiler)
64.4	71.1	67.7	0.0590	0.0348
105.6	109.0	107.3	0.1127	0.0664
122.7	125.6	124.2	0.1749	0.1031
162.7	165.6	164.2	0.4265	0.2509
185.6	187.3	186.4	0.7825	0.4595
187.8	190.0	189.9	0.7762	0.4559
264.4	268.9	266.6	4.956	2.852
-	270.6	270.6	5.00	2.88

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38	-3] Guseva, A.N.; Parnov, E.I.
(2) Water; H ₂ O; [7732-18-5]	Vestn. Mosk. Univ. Khim. <u>1963</u> , 18, 76-9.
VARIABLES:	PREPARED BY:
Temperature: 127-239°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubili	ty of m-xylene in water
<u>t/°C</u> g(1	$100 \text{ g sln}$ $10^4 x_1 \text{ (compiler)}$
127 149	0.031 0.53 0.072 1.22
187 239	0.168 2.85 0.648 11.06
	AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made in	
sealed glass tubes. No detain were reported in the paper.	$n_{\rm D}^{20}$ 1.4974.
	(2) doubly distilled.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Hoegfeldt, E.; Bolander, B.
(2) Water; H ₂ O; [7732-18-5]	Ark. Kemi, <u>1964</u> , 21, 161-86.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	I
The solubility of water in m-Xylene w sln.	as reported to be 0.021 mol (2) $L^{-1}$
The corresponding mass percent and mo compilers are 0.044 g(2)/100 g sln an	÷
The assumption that $1.00 \text{ L} \text{ sln} = 860$	g sln was used in the calculation.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The water determination was carried out according to Johansson's modifi- cation of the Karl Fischer titration in ref 1, 2.	(1) Fluka; 0.3% of ethylbenzene, 0.03% of o-Xylene; purity 99.6%; used as received.
	(2) Not specified.
	ESTIMATED ERROR:
	Temp. ±0.03°C Soly. ±0.001 mol(2) L ⁻¹ sln (type of error not specified)
	REFERENCES: 1. Hardy, C.J.; Greenfield, B.F.;
	Scargill, D. J. Chem. Soc. <u>1961</u> , 90. 2. Johansson, A.
	Sv. Papperstidn. <u>1947</u> , 11B, 124.

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COMPONENTS :	ORIGINAL MEASUREMENTS:			
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3] (2) Water; H ₂ O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.			
VARIABLES:	PREPARED BY:			
Temperature: 10-30°C	A. Maczynski and Z. Maczynska			
EXPERIMENTAL VALUES:				
Solubility of W. <u>t/°C</u> <u>g(2)/100 g sln</u> <u>10</u> 0.0289 <u>20</u> 0.0402 <u>30</u> 0.0536	ater in m-Xylene $\frac{10^{3}x_{2} \text{ (compiler)}}{1.70}$ $2.37$ $3.15$			
AUXILIARY	INFORMATION			
	• · · · · · · · · · · · · · · · · · · ·			
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hy- dride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified.			
	ESTIMATED ERROR: Not specified. REFERENCES:			
	1			

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COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]		Polak, J.; Lu, B.CY.
(2) Water; H ₂ O; [7732-18-5]		Can. J. Chem. <u>1973</u> , 51, 4018-23.
VARIABLES:		PREPARED BY:
Temperature	e: 0-25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL V	/ALUES:	
	Solubility of	m-xylene in water
t/°C	mg(1)/kg(2)	$g(1)/100 g sln 10^{5}x_{1}$ (compiler) (compiler)
0(a)	196(c)	0.0196 3.32
25 (b)	162(c)	0.0162 2.75
	Solubility of	water in m-xylene
t/°C	mg(2)/kg(1)	$g(2)/100 g sln = 10^{3}x_{2}$ (compiler) (compiler)
0(a)	188 (d)	0.0188 1.11
25 (b)	432(e)	0.0432 2.54
	AUXIL	IARY INFORMATION
Approximat with (2) w Hypo-vial teflon coa placed in water bath magnetical the bath f the bath w days, befo for analys The solubi organic la Karl Fisch solubility	ly for 24 hr and left i or 3 days or was kept i ithout stirring for 7 re samples were taken is. lity of water in the yer was determined by er titration and the of hydrocarbon in the r was determined by gas	ESTIMATED ERROR: temp. (a) ± 0.02°C, (b) ± 0.01°C soly. (c) ± 1.7%, (d) ± 4.7%, (e) ± 3.1% (from two or three

36 COMPONENTS: ORIGINAL MEASUREMENTS: (1) m-Xylene; C₈H₁₀; [108-38-3] Sutton, C.; Calder, J.A. (2) Water; H₂O; [7732-18-5] J. Chem. Eng. Data 1975, 20, 320-2. VARIABLES: PREPARED BY: One temperature: 25°C A. Maczynski and Z. Maczynska EXPERIMENTAL VALUES: The solubility of m-xylene in water at 25°C was reported to be 146.0 mg(1)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compilers are 0.01460 g(1)/100 g sln and  $2.48 \times 10^{-5}$ .

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The concentration of (1) in (2) was determined by gas chroma- tography.	(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.			
	(2) distilled.			
	ESTIMATED ERROR:			
	temp. $\pm 0.1^{\circ}C$			
	soly. 1.6 mg(1)/kg(2) (the standard deviation of the			
	<u>mean for six replicates)</u>			
	REFERENCES:			

	37	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3] (2) Water; H ₂ O; [7732-18-5]	Chernoglazova, F.S.; Simulin, Yu.N. Zh. Fiz. Khim. <u>1976</u> , 50, 809. Deposited doc. <u>1976</u> , VINITI 3528-75.	
VARIABLES:	PREPARED BY:	
Temperature: 20-70°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
Solubility of m	-Xylene in Water	
<u>t/°C</u> <u>g(l)/100</u>	g sln $10^5 x_1$ (compiler)	
20 0.016 40 0.022 70 0.038	3.7	
Solubility of W	ater in m-Xylene	
<u>t/°C</u> <u>g(2)/100</u>	g sln $10^3 x_2$ (compiler)	
20 0.034 40 0.067 70 0.190		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The solubility of (1) in (2) was determined by the synthetic method of Fuhner, ref 1. Glass tubes filled with 50-100 mL of (2) were frozen and then (1) was micropipetted. Next, the tubes were sealed and thermo- statted for 6 hrs at 70°C and 72 hrs at 20°C. The solubility was followed visually. The samples were incre- mented at regular steps 0.005 g (1)/ 100 g (2). The mean value from 5-6	<ol> <li>Source not specified; 99.9 purity by glc.</li> <li>Distilled.</li> </ol>	
determinations was adopted.	ESTIMATED ERROR:	
The solubility of (2) in (1) was determined by gas chromatography. The LKhM-7a instrument equipped with a katharometer was employed.	Not specified.	
	REFERENCES :	
	<ol> <li>Fuhner, H.; Chem. Ber. <u>1924</u>, 57, 514.</li> </ol>	
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(l) m-Xylene; C ₈ H ₁₀ ; [108-38-3] (2) Water; H ₂ O; [7732-18-5]	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> ,
2	60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of m-xylene in water a was reported to be 134.0 mg(1)/kg(2) and mole fraction, $x_1$ , calculated by sln and 2.27 x $10^{-5}$ .	The corresponding mass percent
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was determined at	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company;
laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de- tails are given in the paper.	Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 2.0 mg(1)/kg(2) REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Krzyzanowska, T.; Szeliga, J.
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of m-xylene in water a	t 25°C was reported
to be 134.0 mg(1)/kg(2).	
The corresponding mass percent and mo	le fraction, $x_1$ , calculated
by compiler are 0.0134 g(l)/100 g sln	and 2.27 x $10^{-5}$ .
Editor's Note: Based on the results	
systems, uncertainity exists about whe independent of that of Price for the	_
	·····
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways.	(1) not specified.
First, 200 µL of (1) was injected	(2) not specified.
into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1)	
and (2) as above was thermostatted at 70°C and then cooled to 25°C. The	
time required to obtain equilibrium was three weeks. The solubility of	
(1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	
ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame	ESTIMATED ERROR:
ionization detector was used. Sat-	
urated solutions of heptane in (2) were used as standard solutions.	<pre>soly. 3.4 mg(1)/kg(2) (standard deviation from 7-9 determinations).</pre>
	REFERENCES:
L	

COMPONENTS :		ORIGINAL MEASUREMENTS:	
<pre>(1) m-Xylene;</pre>	C ₈ H ₁₀ ; [108-38-3]	Sanemasa, I.; Araki	м.
(2) Water; H ₂ C	0 10	Deguchi, T.; Nagai,	
(2) Macci, "20	, [,,52 10 5]	Bull. Chem. Soc. Jpn.	
			<u></u> ,,
VARIABLES:		PREPARED BY:	· <u>····································</u>
Temperature: 1	.5-45°C	G.T. Hefter	
EXPERIMENTAL VALU	IES:	·····	- <u>.</u>
	The solubility of	m-xylene in water	
t/°C	10 ³ mol(1)/dm ³ sln	g(1)/100 g sln	$10^5 x_{1}$
		(compiler) ^a	(compiler) ^a
15	$1.49 \pm 0.04$	0.0158	2.68
25	$1.52 \pm 0.06$	0.0162	2.75
35	$1.57 \pm 0.10$	0.0168	2.85
45	1.73 ± 0.08	0.0186	3.15
	AUXILIARY	INFORMATION	
METHOD / APPARATUS	PROCEDURE :	SOURCE AND PURITY OF MA	TERIALS:
earlier design described in d 100-200 cm ³ of	is similar to an (ref 2) and is letail in the paper. (2) and 10-20 cm ³ of re placed in separate		
but connected After thermal lished a recir was used to va to transport t containing (2)	thermostatted flasks. equilibrium was estab- culating stream of air porize liquid (1) and the vapor to the flask . Five 10 cm ³ aliquots into separatory	(2) Redistilled; r given.	o further details
funnels. The (2) was then d into chlorofor spectrophotome spectrophotome	concentration of (1) in letermined by extraction m followed by UV- etry. Standards for the etry were prepared by	ESTIMATED ERROR: soly. see table, ty specified. temp. ± 0.1°C.	vpe of error not
	re liquid solutes.	REFERENCES: 1. Kell, G.S. J. Chem. Eng. Date	z <u>1975</u> , 20 , 97.
		2. Sanemasa, I.; P Deguchi, Y.; Na Chem. Lett. 1981	Igai, H.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Sutton, C.; Calder, J.A.
(2) Artificial seawater (ref l)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25.0°C	FREFARED BI;
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of m-xylene in artifi	cial seawater is reported to be
106.0 mg(l)/kg sln. The correspondi	ng mass percent and mole fraction,
$x_1$ calculated by the compiler are 0.	01060 g(1)/100 g sln and 1.85 x $10^{-5}$
assuming the artificial seawater com	
assuming the attiticial seawater com	
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A test tube containing (1) was	SOURCE AND PURITY OF MATERIALS: (1) from either Aldrich Chemical
placed in a flask containing (2) thus allowing for equilibration	Co. or Matheson Coleman and Bell, 99+% pure.
through the vapor phase. The	
saturated solution was extracted with hexane and analyzed by gas	(2) made from doubly distilled water and salts 99+% pure.
chromatography.	
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.6 (std. dev.)
	REFERENCES:
	1. Lyman, J.; Fleming, R.H.;
	J. Mar. Res. <u>1940</u> , 3, 135.
[	

COMPONENTS:	EVALUATOR:	
(2) Water: H_O: [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.	

CRITICAL EVALUATION:

Quantitative solubility data for the p-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the $p-Xylene$ (1) - Water (2) System				
Reference	T/K	Solubility	Method	
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric	
Bohon and Claussen (ref 2)	274-316	(1) in (2)	spectrophotometric	
Pryor and Jentoft (ref 3)	316-577	(1) in (2)	synthetic	
Guseva and Parnov (ref 4)	414-531	(1) in (2)	unspecified	
Hoegfeldt and Bolander (ref 5)	298	(2) in (1)	Karl Fischer	
Polak and Lu (ref 6)	273,298	mutual	GLC, Karl Fischer	
Sutton and Calder (ref 7)	298	(1) in (2)	GLC	
Kirchnerova and Cave (ref 8)	298	(2) in (1)	Karl Fischer	
Price (ref 9)	298	(l) in (2)	GLC	
Krzyzanowska and Szeliga (ref 10)	298	(1) in (2)	GLC	
Sanemasa <i>et al</i> . (ref 11)	288-318	(1) in (2)	spectrophotometric	

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into three parts.

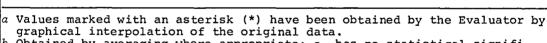
1. SOLUBILITY OF p-XYLENE (1) IN WATER (2)

All the available data on the solubility of p-xylene in water are summarized in Table 2 with the exception of the high temperature data of Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 4) which are discussed in the next section. The 298K datum of Krzyzanowska and Szeliga (ref 10) has also been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 9).

The various data for *p-xylene in water (Table 2) are in only fair agreement* and none of the averaged values are Recommended. At 298K the values cluster around two values: 0.019 (ref 1, 2, 6) and 0.016 g(1)/100g sln (ref 6, 7, 9, 11). Although the values of Bohon and Claussen (ref 2) in well characterized systems are often high this is not sufficient justification for favouring the lower values (ref 7, 9, 11) at this stage. At other temperatures,

(continued next page)

			4	
COMPONEN		EVALUATOR: G.T. Hefter, School of M	lathematical	
<pre>(1) p-Xylene; C₈H₁₀; [106-42-3] (2) Water; H₂0; [7732-18-5]</pre>		and Physical Sciences, Murdoch		
		University, Perth, W.A., Australia.		
		January 1986.		
CRITICAL	EVALUATION: (continued)			
 Т/К		in Water (2) ility values	b	
	Reported values ^a	"Best" value	s (± σ _n )"	
	10 ² g(1)/100g sln	10 ² g(1)/100g sln	$10^{5} x_{1}$	
273	1.55 c (ref 2), 1.64 (ref 6)	1.60 ± 0.05	2.7	
283	1.97 (ref 2)	2.0	3.4	
293	1.96* (ref 2), 1.60* (ref 11)	$1.8 \pm 0.2$	3.1	
298	2.00 (ref 1), 1.98 (ref 2), 1.85 (ref 6), 1.56 (ref 7), 1.57 (ref 9), 1.63 (ref 11)	1.8 ± 0.2	3.1	
303	2.02* (ref 2), 1.68 (ref 11)	1.9 ± 0.2	3.2	
313	2.20* (ref 2), 2.5* (ref 3),	$2.2 \pm 0.3$	3.7	



2.8

3.2

3.6

4.2

4.8

4.7

5.4

6.1

7.1

8.1

1.75 (ref 11)

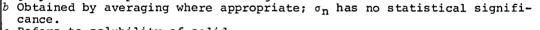
2.8* (ref 3)

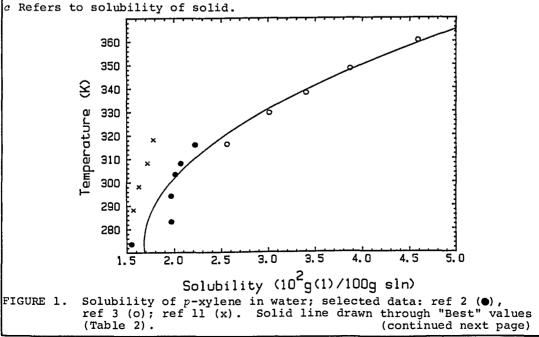
3.2* (ref 3)

3.6* (ref 3)

4.2* (ref 3)

4.8* (ref 3)





323

333

343

353

COMPONENTS:	EVALUATOR:	
(2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.	

agreement is equally poor and at higher temperatures (323-363K) only the values of Pryor and Jentoft (ref 3) are available. Clearly this system warrants further investigation. Selected data have been plotted in Figure 1 which emphasizes the differences among the available data.

Thermodynamic functions derived from various data sets by application of the van't Hoff equation are summarized in Table 3.

TABLE 3: Thermodynamic Functions for the Dissolution ofp-Xylene in Water Derived from Solubility Data

^{∆H} sln kJ mol-1	^{AC} p,sln J K-1 mol-1
3.9	-211
$7.8^{a}_{b}$ 30.4	122 ^a 81 ^b
16.0	210
3.2	11
6.9	204
	kJ mol-1 3.9 7.8 ^a 30.4 ^b 16.0 3.2

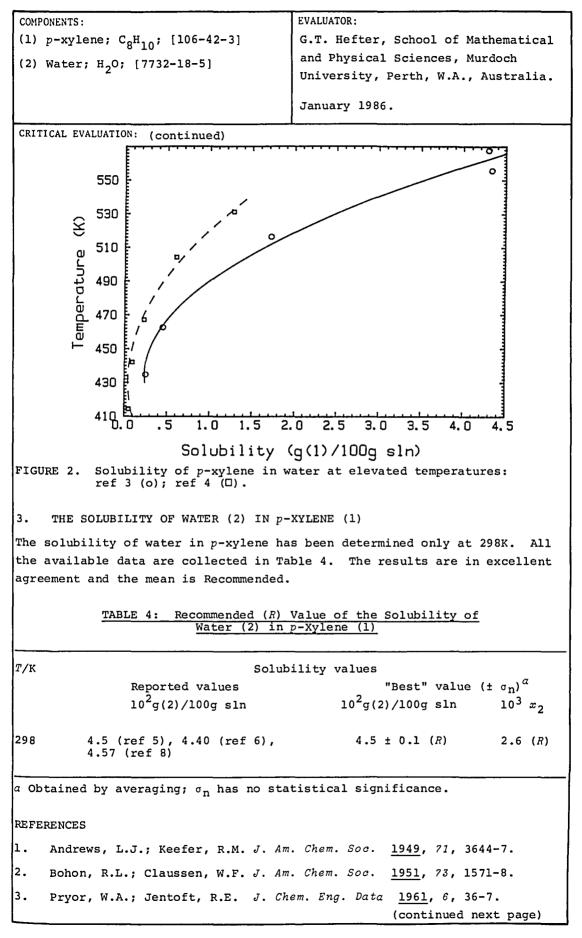
a 316 < T < 360 K b 434 < T < 568 L

Comparison of the thermodynamic data in Table 3 with similar but better characterized hydrocarbon systems (e.g. benzene in water) suggests that none of the solubility data for p-xylene in water are very reliable (including the "Best" values).

2. SOLUBILITY OF p-XYLENE (1) IN WATER (2) AT ELEVATED TEMPERATURES

Solubility data for p-xylene in water at elevated temperatures (*ca.* 400-570K) and system pressure in sealed tubes have been reported by Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 4). The results are plotted in Figure 2 and are clearly in poor agreement. In the absence of confirmatory data it is not possible to know which set is more reasonable. Thermodynamic functions derived from both data sets (Table 3) are in poor agreement and differ markedly from low T values. The interested user is referred to the relevant Data Sheets for the experimental values.

(continued next page)



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COMPONENTS:

(1) p-Xylene; C<sub>8</sub>H<sub>10</sub>; [106-42-3]

(2) Water; H<sub>2</sub>O; [7732-18-5]

University, Perth, W.A., Australia.

January 1986
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REFERENCES (continued)

- 4. Guseva, A.N.: Parnov, E.I. Vestn. Mosk. Univ. Khim. 1963, 18, 76-9.
- 5. Hoegfeldt, E.; Bolander, B. Ark. Kemi <u>1964</u>, 21, 161-86.
- 6. Polak, J.; Lu, B.C.-Y. Can. J. Chem. 1973, 51, 4018-23.
- 7. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.
- 8. Kirchnerova, J.; Cave, G.C.B. Can. J. Chem. 1976, 54, 3909-16.
- Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u>, 60, 213-44; see also Ph.D. Dissertation 1974, University of California, Riverside, CA, U.S.A., <u>1973</u>, quoted in ref 22.
- 10. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.
- 11. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the regression analyses and graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
. –	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of p-Xylene in water a	t 25°C was reported to be
0.0200 g(l)/100 g sln.	
The corresponding mole fraction, $x_1$ , 3.39 x 10 ⁻⁵ .	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant tem-	<ol> <li>Eastman Kodak Co. best grade; fractionally distilled;</li> </ol>
perature bath at 25 C. A sample	b.p. 138.5 C.
(5-20 mL) of the aqueous phase was withdrawn and extracted with a	(2) Not specified.
measured volume of hexane (10-50 mL) by shaking in a glass stoppered	
Erlenmeyer flask. Next, the absorb-	
ance of the hexane phase was measured against a hexane blank on the	
Beckman spectrophotometer.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: (1) p-Xylene;  $C_{gH_{10}}$ ; [106-42-3] Bohon, R.L.; Claussen, W.F. (2) Water; H₂O; [7732-18-5] J. Am. Chem. Soc. <u>1951</u>, 73, 1571-8. VARTABLES . PREPARED BY: G.T. Hefter Temperature: 0.4-42.8°C EXPERIMENTAL VALUES: Solubility of p-xylene in water t/°C  $g(1)/100g \ sln^a$ (compiler) 0.0156^b 0.4 0.0188b 10.0 0.0197 10.0 0.0195 14.9 21.0 0.0197 0.01980 25.0 25.6 0.0199

 a  Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical This gave a solubility of g(1)/L sln which was then densities. converted to q(1)/100q sln by assuming a solution density of 1.00 kg/L.

0.0201

0.0204

0.0207

0.0207

0.0222

 $10^{5}x_{1}$ 

(compiler) 2.64^b

3.19^b

3.34

3.31

3.34

3.360

3.37 3.41

3.46 3.51

3.51

3.76

^bData refer to solubility solid (1) in (2).

30.2 30.3

34.9 35.2

42.8

^cGiven in the original paper as 0.198g(1)/L sln.

AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE : SOURCE AND PURITY OF MATERIALS: Eastman Kodak Co., purified by recrystallization from ethanol, A round-bottomed flask containing. about 4 mL of (1) and 400 mL of (2) washing, filtering through was evacuated, suspended in a thermostat, shaken for 24h and then silica gel then distilling. allowed to settle for at least another Purity was determined by 24h. Next, desired quantities of the refractometry (no details given). water layer were syphoned into 6 (2) Air-free conductivity water, no glass-stoppered Erlenmeyer flasks. other details given. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of ESTIMATED ERROR: the samples were inserted into a Temp. ± 0.02°C quartz cuvette and measured in a Soly. ± 0.5% relative Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette. **REFERENCES:** 

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Pryor, W.A.; Jentoft, R.E.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1961</u> , 6, 36-7.
VARIABLES:	PREPARED BY:
Temperature: 43.0-294.5°	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

### Solubility of p-xylene in water

	t/°C		з	
Cloud point appears	Cloud point disappears	Midpoint	$\frac{10^{3}x_{1}}{10^{3}}$	g(l)/100 g sln (compiler)
42.8	43.3	43.0	0.0434	0.0256
54.4	58.3	56.4	0.0510	0.0301
61.7	68.3	65.0	0.0576	0.0340
73.9	76.7	75.3	0.0656	0.0387
85.0	89.4	87.2	0.0779	0.0459
161.7	163.3	162.5	0.4264	0.2508
186.7	189.5	188.1	0.7686	0.4514
241.6	244.9	243.2	2.9555	1.7174
280.5	284.4	282.5	7.6238	4.3326
291.6	298.3	294.5	7.5407	4.2871

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Mixture of (1) and (2) were carefully weighed into glass ampoules. The ampoules were sealed allowing just enough space for thermal expansion. The ampoule, observed through a telescope from behind a safety barrier, was suspended in a 4-liter stirred silicone oil bath, and the bath was heated until the (1) dis- solved. On cooling, a cloud of fine (1) droplets appeared, making the suspension opaque. The temperature was raised until the cloud dis- appeared. The cycle was repeated three to four times until reliable	<ol> <li>source not specified; 99.1% by freezing point; main impurities are isomeric xylenes; used as received.</li> <li>not specified.</li> </ol> ESTIMATED ERROR: not specified.
atures for the cloud were recorded.	REFERENCES :

-	-
n	4
-	

COMPONENTS :			ORIGIN	AL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]		Gusev	a, A.N.; Parnov, E.I.	
(2) Water; H ₂ O; [7732-18-5]		Vestn. Mosk. Univ. Khim. <u>1963</u> , 18, 76-9.		
VARIABLES: Temperature	e: 141 - 25	8°C	PREPARI A. M	ED BY: aczynski and Z. Maczynska
	50 <u>t/°C</u>	g(1)/100 g	-	in water 10 ⁴ x ₁ (compiler)
	141 169 194 231 258	0.049 0.096 0.231 0.607 1.283		0.83 1.63 3.93 10.34 22.00

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The measurements were made in sealed glass tubes. No details were reported in the paper.	(1) source not specified; n _D ²⁰ 1.4958.	
	(2) doubly distilled.	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:		
	ORIGINAL MERSUREMIS.		
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Hoegfeldt, E.; Bolander, B.		
(2) Water; H ₂ O; [7732-18-5]	Ark. Kemi, <u>1964</u> , 21, 161-86.		
2			
VARIABLES:	PREPARED BY:		
One temperature: 25°C	A. Maczynski and Z. Maczynska		
	4		
EXPERIMENTAL VALUES:			
The solubility of water in p-Xylene wa	as reported to 0.022 mol(2) $L^{-1}$ sln.		
The corresponding mass percent and mol fraction, $x_2$ , calculated by the compilers are 0.045 g(2)/100 g sln and 0.0027.			
$\frac{1}{2}$	0.0027.		
The assumption that 1.00 L sln = $857$ c	g sln was used in the calculation.		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The water determination was carried	(1) Fluka; 0.04% of ethylbenzene;		
out according to Johansson's modifi- cation of the Karl Fischer titration	purity 99.8%; used as received.		
described in ref 1, 2.	(2) Not specified.		
	ESTIMATED ERROR:		
	Temp. ±0.3°C		
	Soly. ±0.002 mol(2) L ⁻¹ sln (type of error not specified)		
	REFERENCES:		
	<ol> <li>Hardy, C.J.; Greenfield, B.F.; Scargill, D.</li> </ol>		
	J. Chem. Soc. 1961, 90.		
	2. Johansson, A. Sv. Papperstidn. <u>1947</u> , 11B, 124.		

 COMPONENTS:
 ORIGINAL MEASUREMENTS:

 (1) p-Xylene; C₈H₁₀; [106-42-3]
 Polak, J.; Lu, B.C.-Y.

 (2) Water; H₂O; [7732-18-5]
 Can. J. Chem. <u>1973</u>, 51, 4018-23.

 VARIABLES:
 PREPARED BY:

 Temperature: 0-25°C
 A. Maczynski and Z. Maczynska

## EXPERIMENTAL VALUES:

Solubility of p-xylene in water

t/°C	mg(1)/kg(2)	g(l)/100 g sln (compiler)	10 ⁵ x1 (compiler)
0†(a)	164(c)	0.0164	2.78
25 (b)	185(c)	0.0185	3.14

The solubility of water in p-xylene at 25°C was reported to be 440 mg(l)/kg(2). The corresponding mass percent and mole fraction,  $x_2$ , calculated by the compilers are 0.0440 g(2)/100 g sln and 2.59 x  $10^{-3}$ .

a-c See "Estimated Error" †p-xylene was at supercooled liquid state.

AUXILIARY INFORMATION METHOD / APPARATUS / PROCEDURE : SOURCE AND PURITY OF MATERIALS: (1) Eastman Organics, pure grade Approximately 50 mL of (1) together with (2) were placed in a 125 mL reagent; shaken three times with distilled water. Hypo-vial which was closed with a teflon coated rubber septum and (2) distilled. placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis. ESTIMATED ERROR: The solubility of water in the organic layer was determined by Karl Fischer titration and the temp. (a)  $\pm$  0.02°C, (b)  $\pm$  0.01°C soly. (c) ± 1.7% (from two or three solubility of hydrocarbon in the determinations) water layer was determined by gas chromatography. **REFERENCES:** 

COMPONENTS:	ORIGINAL MEASUREMENTS:
	Kirchnerova, J.; Cave, G.C.B.
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	
(2) Water; H ₂ O; [7732-18-5]	Can. J. Chem. <u>1974</u> , 54, 3909-16.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
one cemperature: 25 C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of water in p-xylene at 25°C was reported to be 0.0217 mol(2)/L and $x_2 = 0.00269$ . The corresponding mass percent calculated by the compilers is 0.0457 g(2)/l00 g sln.	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Approximately 50 mL of (1) was placed in the equilibration vessel. A test tube containing 6 mL of (2) was then placed in the vessel so that the rim of the test tube rested against the upper inside wall of the vessel. The vessel was then stoppered, placed inside a plastic bag, and the jacketed vessel was emersed up to its neck in a water thermostat. Trials had shown that the stoichiometric concentration of (1) in (2) became constant within 2 days. The stoichiometric concentration of water was determined by a conventional Karl Fischer dead-stop back-titration.	<pre>(1) Fisher 277; purified by double crystallization. (2) not specified. ESTIMATED ERROR: temp. ± 0.1°C soly. 0.0002 mol(2) dm⁻³ sln (standard deviation from 5 determinations). REFERENCES:</pre>

```
COMPONENTS:
 ORIGINAL MEASUREMENTS:
 (1) p-Xylene; C<sub>8</sub>H<sub>10</sub>; [106-42-3]
 Sutton, C.; Calder, J.A.
 J. Chem. Eng. Data 1975, 20, 320-2.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
VARIABLES:
 One temperature: 25°C
```

PREPARED BY: A. Maczynski and Z. Maczynska

#### EXPERIMENTAL VALUES:

The solubility of p-xylene in water at 25°C was reported to be 156.0 mg(1)/kg(2). The corresponding mass percent and mole fraction,  $\boldsymbol{x}_{1},$  calculated by the compilers are 0.01560 g(l)/100 g sln and  $2.65 \times 10^{-5}$ .

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The concentration of (1) in (2) was determined by gas chroma- tography.	<ul> <li>Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.</li> </ul>		
	(2) distilled.		
	ESTIMATED ERROR: temp. ± 0.1°C soly. 1.6 mg(1)/kg(2) (the standard deviation of the mean for six replicates)		
	REFERENCES:		

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

# EXPERIMENTAL VALUES:

The solubility of p-xylene in water at 25°C and at system pressure was reported to be 157.0 mg(l)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 0.0157 g(l)/ 100 g sln and 2.66 x 10⁻⁵.

AUXILIARY INFORMATION         METHOD/APPARATUS/PROCEDURE:       SOURCE AND PURITY OF MATERIALS:         The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.       (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.         (2) distilled.       (2) distilled.         ESTIMATED ERROR:       temp. ± 1°C soly. ± 1.0 mg(1)/kg(2)         REFERENCES:       REFERENCES:		
<ul> <li>The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.</li> <li>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>(2) distilled.</li> <li>(2) distilled.</li> <li>(2) distilled.</li> <li>(2) distilled.</li> </ul>	AUXILIARY	INFORMATION
	laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de-	<ul> <li>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>(2) distilled.</li> </ul> ESTIMATED ERROR: temp. ± 1°C soly. ± 1.0 mg(1)/kg(2)

```
COMPONENTS:
(1) p-Xylene; C8H10; [106-42-3]
(2) Water; H20; [7732-18-5]ORIGINAL MEASUREMENTS:
Krzyzanowska, T.; Szeliga, J.
Nafta (Katowice), 1978, 12, 413-7.VARIABLES:
One temperature: 25°CPREPARED BY:
M.C. Haulait-Pirson
```

#### EXPERIMENTAL VALUES:

The solubility of p-xylene in water at 25°C was reported to be 157.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 0.0157 g(1)/100 g sln and 2.66 x  $10^{-5}$ .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150-mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>		
	REFERENCES :		

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) $n = Xy = 0$ (106-42-3)	Sanemasa, I.; Araki, M.;	
<pre>(1) p-Xylene; C₈H₁₀; [106-42-3] (2) Water; H₂O; [7732-18-5]</pre>	Deguchi, T.; Nagai, H.	
$(2)$ water; $n_20$ ; $[7752-10-5]$	Bull. Chem. Soc. Jpn. <u>1982</u> , 55, 1054-62.	
	<u>220-</u> , 00, 101 02.	
VARIABLES:	PREPARED BY:	
Morrowsturgs 15, 45%C	G.T. Hefter	
Temperature: 15-45°C	G.I. NEILEI	
EXPERIMENTAL VALUES:		
The solubility	of p-xylene in water	
$t/^{\circ}C$ 10 ³ mol(1)/dm ³ sln	$\begin{array}{c} g(1)/100 \ g \ sln \\ (compiler)^{a} \end{array}  \begin{array}{c} 10^{5} \ x_{1} \\ (compiler)^{a} \end{array}$	
15 1.48 ^b	0.0157 2.67	
25 1.53 ± 0.07	0.0163 2.76	
35 1.61 ± 0.08	0.0172 2.92	
45 1.66 ± 0.05	0.0178 3.02	
AUXILI	ARY INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab lished a recirculating stream of ai was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ alique were withdrawn into separatory	<ul> <li>(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.</li> <li>(2) Redistilled; no further details given.</li> </ul>	
funnels. The concentration of (1) (2) was then determined by extracting into chloroform followed by UV- spectrophotometry. Standards for t spectrophotometry were prepared by weight from pure liquid solutes.	on soly. see table, type of error not	
	1. Kell, G.S. J. Chem. Eng. Data <u>1975</u> , 20 , 97.	
	<ol> <li>Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. Chem. Lett. <u>1981</u>, 225-8.</li> </ol>	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Sutton, C.; Calder, J.A.
(2) Artificial seawater (ref 1)	J. Chem. Eng. Data <u>1975</u> , 20, <b>320-2</b> .
VARIABLES: One temperature: 25.0°C	PREPARED BY:
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of p-xylene in artifi	cial seawater is reported to be
110.9 mg(1)/kg sln. The correspondi	
	01109 g(1)/100 g sln and 1.93 x $10^{-5}$
assuming the artificial seawater com	
assuming the artificial seawater ton	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A test tube containing (1) was placed in a flask containing (2)	(1) from either Aldrich Chemical Co. or Matheson Coleman and
thus allowing for equilibration through the vapor phase. The	Bell, 99+% pure.
saturated solution was extracted with hexane and analyzed by gas	(2) made from doubly distilled water and salts 99+% pure.
chromatography.	
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.9 (std. dev.)
	REFERENCES:
	<ol> <li>Lyman, J.; Fleming, R.H.; J. Mar. Res. <u>1940</u>, 3, 135.</li> </ol>

COMPONENTS :	EVALUATOR:
<pre>(1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the ethylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of theEthylbenzene (1) - Water (2) System

Reference	T/K	Solubility	Method	
Fühner (ref 1)	288	(1) in (2)	titration	
Andrews and Keefer (ref 2)	298	(1) in (2)	spectrophotometric	
Klevens (ref 3)	298	(l) in (2)	spectrophotometric	
Bohon and Claussen (ref 4)	273-316	(l) in (2)	spectrophotometric	
Filippov and Furman (ref 5)	291-323	(2) in (1)	synthetic	
Morrison and Billett (ref 6)	298	(l) in (2)	analytical	
Jones and Monk (ref 7)	298-308	(2) in (1)	radiotracer	
McAuliffe (ref 8)	298	(l) in (2)	GLC	
Guseva and Parnov (ref 9)	338-507 ^a	(1) in (2)	unspecified	
Englin <i>et al</i> . (ref 10)	283-303	(2) in (1)	analytical	
McAuliffe (ref ll)	298	(1) in (2)	GLC	
Polak and Lu (ref 14)	273,298	mutual	GLC, Karl Fischer	
Brown and Wasik (ref 15)	278-293	(l) in (2)	chromatographic	
Sutton and Calder (ref 16)	298	(l) in (2)	GLC	
Price (ref 17)	298	(l) in (2)	GLC	
Korenman and Aref'eva (ref 18	3) 293	(1) in (2)	titration	
Korenman and Aref'eva (ref 19	9) 298	(l) in (2)	titration	
Krzyzanowska and Szeliga (ref 20)	298	(1) in (2)	GLC	
Sanemasa <i>et al</i> . (ref 21,22)	288-318	(l) in (2)	spectrophotometric	
Sanemasa <i>et al</i> . (ref 23)	298	(1) in (2)	spectrophotometric	
Heidman <i>et al</i> . (ref 24)	311-568 ^a	mutual	GLC, Karl Fischer	

a Pressure also varied, see Table 6.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Critical phenomena at high pressures have been reported by Alwani and Schneider (ref 12) and Roof (ref 13) and are discussed along with the high pressure solubility data (ref 9, 24) in Section 3 below. For convenience, further discussion of this system will be divided into three parts.

(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

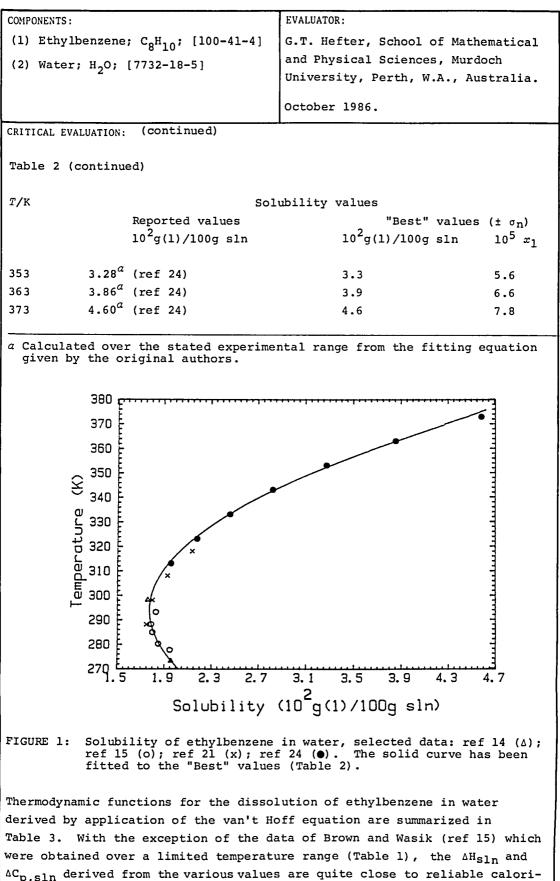
In the tables which follow values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original authors' experimental data. "Best" values have been obtained by averaging all non-rejected data. Standard deviations  $(\sigma_n)$  have been included as a convenient measure of the spread of experimental results: they do not have any statistical significance.

## 1. SOLUBILITY OF ETHYLBENZENE (1) IN WATER (2)

Of the data available on the solubility of ethylbenzene in water, values of Bohon and Claussen (ref 4) and Korenman and Aref'eva (ref 18) have been rejected because they are significantly higher (by about 10%) than all other studies. The value of Price (ref 17) at 298K is markedly lower than all other studies and is also rejected. The datum of Krzyzanowska and Szeliga (ref 20) has been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 17). The remaining data are summarized in Table 2 and are generally in excellent agreement even though few studies have covered the same temperature range (which has limited the number of Recommended values). Selected data are also plotted in Figure 1.

T/K	Solubilit	y values	
	Reported values	"Best" values	
	10 ² g(1)/100g sln	10 ² g(1)/100g sln	10 ⁵ x ₁
273	1.97 (ref 14)	2.0	3.4
283	1.84* (ref 15)	1.8	3.1
293	1.84* (ref 15), 1.77 (ref 21)	1.81 ± 0.04 (R)	3.07 (R)
298	<pre>1.68 (ref 2), 1.75 (ref 3), 1.65 (ref 6), 1.59 (ref 8), 1.52 (ref 11), 1.77 (ref 14), 1.61 (ref 16), 1.8 (ref 19), 1.81 (ref 21), 1.69 (ref 22), 1.72 (ref 23)</pre>	1.69 ± 0.09 (R)	2.87 ( <i>R</i> )
303	1.86* (ref 21)	1.9	3.2
313	2.03* (ref 21), 1.97 ^{<i>a</i>} (ref 24)	$2.00 \pm 0.03 (R)$	3.39 (R)
323	2.19 ^{<i>a</i>} (ref 24)	2.2	3.7
333	2.47 ^{<i>a</i>} (ref 24)	2.5	4.2
343	2.83 ^{<i>a</i>} (ref 24)	2.8	4.8
		(Table 2 continued )	next nage)
		(Table 2 Continued )	mexic page/

TABLE 2:	Recommended (R)	) and Tentative	Values of	the Solubility
	of Ethy	lbenzene (l) in	Water (2)	



metric values reported for the dissolution of benzene in water. This gives added confidence to the solubility data in Table 2. (continued next page)

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COMPONENTS:

(1) Ethylbenzene; C<sub>8</sub>H<sub>10</sub>; [100-41-4]

(2) Water; H<sub>2</sub>O; [7732-18-5]

(2) Water; H<sub>2</sub>O; [7732-18-5]

(3) Cotober 1986.
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# TABLE 3: Thermodynamic Functions for the Dissolution of Ethylbenzene in Water Derived from Solubility Data

^{AH} sln kJ mol-1	ΔC _{p,sln} . J K ⁻¹ mol ⁻¹
11.9	1123
3.6	319
3.9	230
4.5	213
2.1	275
	kJ mol-l ll.9 3.6 3.9 4.5

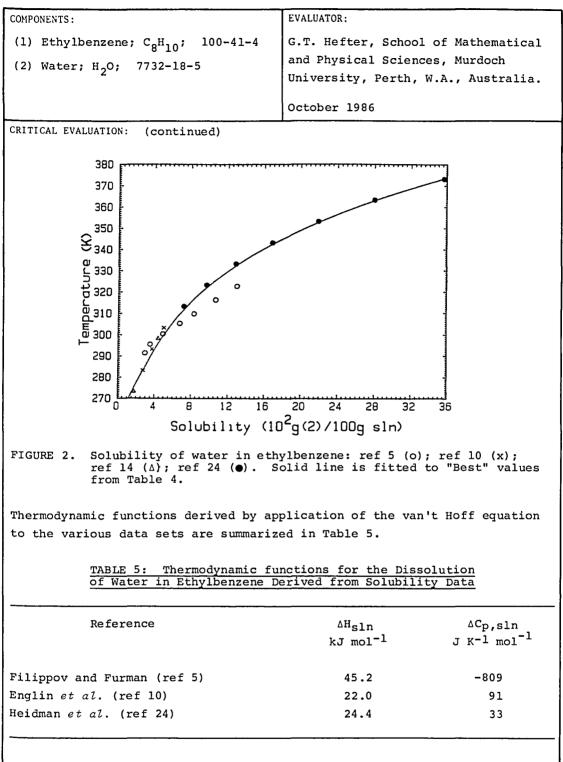
2. SOLUBILITY OF WATER (2) IN ETHYLBENZENE (1)

With the exception of the data of Jones and Monk (ref 7) which are reported in v/v fractions, all the available values for the solubility of water in ethylbenzene are summarized in Table 4 below. Unfortunately, few of the determinations cover the same temperature range. Where comparison is possible at lower temperatures ( $T \leq 298$ K) independent determinations are in reasonable agreement. At higher temperatures (T > 298K) the values of Filippov and Furman (ref 5) and Heidman *et al.* (ref 24) show an increasing divergence with increasing temperature (Figure 2).

TABLE 4: Recommended (R) and Tentative Values of the Solubilityof Water (2) in Ethylbenzene (1)

T/K	Solubilit	Solubility values					
	Reported values	"Best" value					
	10 ² g(2)/100g sln	10 ² g(2)/100g sln	10 ³ x ₂				
273	1.78 (ref 14)	1.8	1.1				
283	2.75 (ref 10)	2.8	1.7				
293	3.3* (ref 5), 3.73 (ref 10)	3.5 ± 0.2	2.1				
298	4.2* (ref 5), 4.4* (ref 10), 4.42 (ref 14)	4.3 ± 0.1 (R)	2.5 (R)				
303	5.9* (ref 5), 5.02 (ref 10)	5.5 ± 0.5	3.2				
13	9.6* (ref 5), 7.2 ^{$\alpha$} (ref 24)	8 ± 1	5				
23	13.3* (ref 5), 9.68 ^{<i>a</i>} (ref 24)	11 ± 2	6				
333	12.9 ^{<i>a</i>} (ref 24)	13	8				
343	16.9 ^{<i>a</i>} (ref 24)	17	10				
353	21.9 ^{<i>a</i>} (ref 24)	22	13				
363	$28.0^{a}$ (ref 24)	28	17				
373	35.6 ^{<i>a</i>} (ref 24)	36	21				

a Calculated over the stated experimental range by the fitting equation given by the original authors. (continued next page)



The thermodynamic functions derived from the data of both Englin *et al.* (ref 10) and Heidman *et al.* (ref 24) are comparable to those obtained for related, well characterized systems (*e.g.* water in benzene) whereas the values of Filippov and Furman (ref 5) are not. Further investigation of this system is clearly warranted.

COMPONENTS:	EVALUATOR:
<pre>(1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia.
	October 1986.

3. MUTUAL SOLUBILITIES OF ETHYLBENZENE (1) AND WATER (2) AT ELEVATED TEMPERATURES

To clarify the relationship between the phases in equilibrium it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram for this system. On such a diagram (Figure 3) phases with the same value of pressure and temperature but different composition will be located at the same point. The general typology of the phase diagram of this system is similar to that of benzene + water (except that the vapor pressure of ethylbenzene is considerably less than that of benzene). Ethylbenzene + water has type III phase behaviour (using Scott and von Konynenberg's classification (ref 25, 26). This type of phase behaviour is characterized by two critical loci, with one starting at the critical point of the pure component with the higher critical temperature (water in this case) and eventually approaching high pressures. The other critical locus starts at the critical point of the other pure component (ethylbenzene) and ends on a three phase (liquid-liquid-vapor) line at a critical end point.

The p-T projection of the p-T-x diagram for this system is shown schematically in Figure 3.

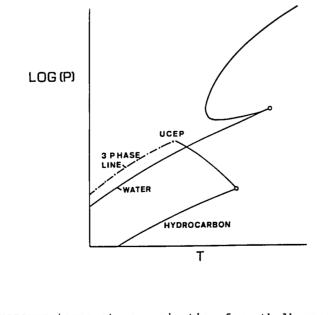


FIGURE 3. Pressure-temperature projection for ethylbenzene/water.

COMPONENTS:	EVALUATOR:
<pre>(1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia.
	October 1986.

It is important to note that the three phase line on a p-T projection corresponds to three lines on the p-T-x diagram. In the region above the three phase line on the p-T projection, the pressure is greater than the vapor pressure and then a maximum of two liquid phases is possible. There may be one or two liquid phases depending on the overall composition. To the left of the critical line starting at the least volatile component it is possible to have one or two phases present depending on the overall composition.

Solubilities in the ethylbenzene + water system have been studied at elevated pressures in the publications listed in Table 6.

TABLE 6:	Solubility	Studies	of the	Ethylbenzene	(1)	- Water (2)
	Sy	stem at	Elevated	l Pressures		

Reference	p/kPa	T/K	Solubility
Guseva and Parnov (ref 9)	_a	338-507	(1) in (2)
Alwani and Schneider (ref 12)	1.8-2.0 b	348-387 b	critical locus
Roof (ref 13) Heidman <i>et al</i> . (ref 24)	- 0.1-10.7 ^c	- 311-568	mutual
	012 2001	011 000	mutuur

a Unspecified but presumably at pressures on the three phase line. b Critical point of unknown composition.

c Along three phase line.

The data of Guseva and Parnov (ref 9) are thought to be unreliable. The solubilities reported by these workers are considerably larger than values obtained by other workers for the systems water + benzene, + hexane, + ethylcyclohexane and + octane. The data of Heidman *et al.* (ref 24) are classified as Tentative for measurements along the three phase line. However, it should be pointed out that there is some discrepancy between the critical end point properties (574.3K, 11.2 MPa) reported by Roof (ref 13) and those reported by Heidman *et al.* (568.1K, 10.68 MPa). Nevertheless, the thermodynamic functions derived from the data of Heidman *et al.* (Table 3) and also with those of related hydrocarbons (*e.g.* benzene in water).

Alwani and Schneider (ref 12) have reported values of the critical properties along the critical curve starting at the critical point of ethylbenzene (cf. Figure 3).

COMPONENTS: EVALUATOR: G.T. Hefter, School of Mathematical (1) Ethylbenzene; C₈H₁₀; [100-41-4] and Physical Sciences, Murdoch University, Perth, W.A., Australia. (2) Water; H₂O; [7732-18-5] October 1986 CRITICAL EVALUATION: (continued) REFERENCES 1. Fühner, H. Chem. Ber. 1924, 57, 510-5. 2. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1950</u>, 72, 5034-7. 3. Klevans, H.B. J. Phys. Chem. 1950, 54, 283-98. 4. Bohon, R.L.; Claussen, W.F. J. Am. Chem. Soc. 1951, 73, 1571-8. 5. Filippov, T.S.; Furman, A.A. Zh. Prikl. Khim. 1952, 25, 895-7. 6. Morrison, T.J.; Billett, F. J. Chem. Soc. 1952, 3819-22. 7. Jones, J.R.; Monk, C.B. J. Chem. Soc. 1963, 2633-5. McAuliffe, C. Nature 1963, 200, 1092-3. 8. 9. Guseva, A.N.; Parnov, E.I. Zh. Fiz. Khim. 1964, 38, 805-6. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6. 10. 11. McAuliffe, C. J. Phys. Chem. <u>1966</u>, 70, 1267-75. Alwani, Z.; Schneider, G.M. Ber. Bunsenges. Phys. Chem. 1969, 70, 294-301. 12. 13. Roof, J.G. J. Chem. Eng. Data 1970, 15, 301-3. 14. Polak, J.; Lu, B.C.-Y. Can. J. Chem. 1973, 51, 4018-23. 15. Brown, R.L.; Wasik, S.P. J. Res. Natl. Bur. Stds. A. 1974, 78, 453-60. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2. 16. 17. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44; see also Price, L.C. Ph.D. Dissertation, Univ. California, Riverside, CA, U.S.A., 1973, quoted in ref 22. Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977,04.05. 18. 19. Korenman, I.M.; Aref'eva, R.P. Zh. Prikl. Khim. 1978, 51, 957-8. 20. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7. 21. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Chem. Lett. 1981, 225-8. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 22. 1982, 55, 1054-62. 23. Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. Bull. Chem. Soc. Jpn. 1984, 57, 1539-44. 24. Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. A.I.Ch.E.J. 1985, 31, 376-84. 25. Scott, R.L.; van Konynenburg, P.H. Phil. Trans. Roy. Soc., London 1980, A298, 495. 26. Hicks, C.P.; Young, C.L. Chem. Rev. 1975, 75, 119.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Fuhner, H.
(2) Water; H ₂ O; [7732-18-5]	Ber. Dtsch. Chem. Ges. <u>1924</u> , 57, 510-5.
VARIABLES:	PREPARED BY:
One temperature: 15°C	A. Maczynski, Z. Maczynska and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wate 0.014 g(l)/100 g sln.	er at 15°C was reported to be
The corresponding mole fraction, $x_1$ , $(2.4 \times 10^{-5})$ .	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to	(1) Source not specified; commer- cial grade; used as received.
50, 100, or 1000 cm ³ (2) until a completely clear solution was no	(2) Not specified.
longer obtained at the experimental temperature.	
	ESTIMATED ERROR:
	Not specified.
	PEEPENOVC.
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wate	er at 25°C was reported to be
0.0168 g(1)/100 g sln.	
The corresponding mole fraction, $x_1$ , 2.85 x 10 ⁻⁵ .	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant tem- perature bath at 25°C. A sample	(1) Eastman Kodak Co. white label; fractionally distilled; b.p. 136.0°C.
(5-20 mL) of the aqueous phase was withdrawn and extracted with a	(2) Not specified.
measured volume of hexane (10-50 mL) by shaking in a glass stoppered	
Erlenmeyer flask. Next, the absorb- ance of the hexane phase was mea-	
sured against a hexane blank on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

Parana and a second	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	L
The solubility of ethylbenzene in wat 0.175 g(l) L ⁻¹ sln and 0.00164 mol(l	er at 25°C was reported to be ) L ⁻¹ sln.
The corresponding mass percent and mo compiler are 0.0175 g(l)/100 g sln an	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

70	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Bohon, R.L.; Claussen, W.F.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1951</u> , 73, 1571-8.
VARIABLES:	
Temperature: 0.4-42.8°C	PREPARED BY: G.T. Hefter
Temperature: 0.4-42.8°C	G.I. neiter
EXPERIMENTAL VALUES:	
	ylbenzene in water 00g sln ^a $10^5 x_1$
(com	piler) (compiler)
	0219 3.71 0213 3.61
	0207 3.51
	0207 3.51 2202 <i>h</i>
	0208 ^b 3.53 0209 3.54
30.2 0.	0211 3.58
	0221 3.75 0231 3.92
Solubilities of (1) in (2) were repo measurements. Solubilities were cal- Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(1)/100g sln by assumin ^b Given in the original paper as 0.208	th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Filippov, T.S.; Furman, A.A.
(2) Water; H ₂ O; [7732-18-5]	Zh. Prikl. Khim. <u>1952</u> , 25, 895-7.
2	
VARIABLES:	PREPARED BY:
	) Maggunghi and 5 Maggungha
Temperature: 18.2-49.5°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of water	in ethylbenzene
t/°C g(2)/100 g slr	$10^3 x_2$ (compiler)
18.2 0.0296 18.3 0.0308	1.74 1.81
19.7 0.0327 22.3 0.0352	1.92 2.07
23.4 0.0360	2.12
24.2 0.0388 27.2 0.0494	2.28 2.91
29.8 0.0595	3.50
31.6 0.0648 32.1 0.0679	3.81 4.05
34.2 0.0745	4.38
35.1 0.0777 36.6 0.0835	4.56 4.90
38.8 0.0917	5.38
41.5 0.1005 43.1 0.1070	5.90 6.27
47.2 0.1225	7.18
49.5 0.1300	7.62
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Weighed amounts of both components	(1) source unspecified; distilled;
were placed in glass tubes, 40 mm	no turbidity if cooled to
across and 65 mm long, and shaken. Clear and cloud points were ob-	-10 or -20°C.
served 5-6 times to within 0.2-	(2) twice distilled.
0.3°C.	
	ESTIMATED ERROR:
	<pre>temp: ± 0.3°C soly: not specified</pre>
	REFERENCES:
1	
	l

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Morrison, T.J.; Billett, F.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Soc. <u>1952</u> , 3819-22.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wat 0.00155 mol(1)/1000 g(2). The corresponding mass percent and mo by compilers are 0.0165 g(1)/100 g sl	ble fraction, $x_1$ , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
After an excess of (1) had been shaken with about 1 dm ³ of (2) for about a week, a known volume of saturated solution was made slightly alkaline, and a stream of pure air passed through to drive off the (1). After passage through a silica tube packed with cupric oxide and heated to redness, the (2) was removed by concentrated sulfuric acid and calcium chloride and the carbon dioxide absorbed and weighed in soda-asbestos. The precautions usual in organic combustions were taken.	<pre>(1) source not specified; purest obtainable material; distilled; purity not specified. (2) not specified. ESTIMATED ERROR: temp. ± 0.1°C soly. ± 1% (mean of large numbers</pre>
	of determinations)

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Jones, J.R.; Monk, C.B.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Soc. <u>1963</u> , 2633-5.
VARIABLES:	PREPARED BY:
Temperature: 25-35°C	A. Maczynski, Z. Maczynska and
	A. Szafranski
EXPERIMENTAL VALUES:	
	er in Ethylbenzene
<u>t/°C</u>	$10^4$ mL (2)/mL (1)
25 30	3.7 4.3
35	5.3
AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl ₂ and fractionally distilled
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for nin 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter-	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl ₂ and fractionally distilled
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli-	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl ₂ and fractionally distilled
METHOD/APPARATUS/PROCEDURE:	<pre>SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl₂ and fractionally distilled (2) Not specified.</pre>
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	<pre>SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl₂ and fractionally distilled (2) Not specified. ESTIMATED ERROR:</pre>
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- guot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	<pre>SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl₂ and fractionally distilled (2) Not specified.</pre>
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	<pre>SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl₂ and fractionally distilled (2) Not specified.  ESTIMATED ERROR: Soly, ±5% to ±1%</pre>
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	<pre>SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl₂ and fractionally distilled (2) Not specified. ESTIMATED ERROR: Soly. ±5% to ±1%     (average deviation)</pre>
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	<pre>SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl₂ and fractionally distilled (2) Not specified. ESTIMATED ERROR: Soly. ±5% to ±1%     (average deviation)     .</pre>

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Water; H₂0; [7732-18-5]</pre>	McAuliffe, C. Nature (London) 1963, 200, 1092-3.
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wat 0.0159 g(l)/100 g sln.	er at 25°C was reported to be
The corresponding mole fraction, $x_1$ , 2.70 x 10 ⁻⁵ .	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker	<pre>(1) Phillips Petroleum Co.; 99+%; used as received.</pre>
or stirring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon- saturated water was injected directly into a gas liquid chromatograph.	(2) Distilled.
Theo a gas figura chromatograph.	
	ESTIMATED ERROR: Temp. ±1.5°C
	Soly. 0.0008 (std. dev. of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Guseva, A.N.; Parnov, E.I.
(2) Water; H ₂ O; [7732-18-5]	Zh. Fiz. Khim. 1964, 38, 805-6.
VARIABLES:	DEBARED NV.
Temperature: 115.0 - 233.5°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of ethylbe	nzene in water
<i>t/°C</i> g(1)/100 g sln	$10^4 x_1$ (compiler)
115.0 0.0513	0.871
140.5 0.119 170.5 0.355	2.02 6.04
210.0 0.661	11.27
233.5 1.129	19.33
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The measurements were made in	(1) not specified.
sealed glass tubes. No details were reported in the paper.	(2) not specified.
	· · · ·
	ESTIMATED ERROR:
	ESTIMATED ERROR:
	not specified.
	REFERENCES :
l	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4] (2) Water; H ₂ O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	l
Solubility of Wat	er in Ethylbenzene
<u>t/°C</u> <u>g(2)/100 g sl</u>	$\frac{10^3 x_2 (\text{compiler})}{10^3 x_2 (\text{compiler})}$
10         0.0275           20         0.0373           30         0.0502	1.62 2.19 2.95
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	<ul><li>(1) Not specified.</li><li>(2) Not specified.</li></ul>
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
VARIABLES:	
	PREPARED BY: A. Maczynski, Z. Maczynska, and
One temperature: 25°C	A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in water at 25°C was reported to be 152 g(1)/10 ⁶ g(2). The corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are 0.0152 g(1)/100 g sln and 2.57 x 10 ⁻⁵ .	
	·
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromato- graphed in conjunction with a flame- ionization detector.	<ul> <li>(1) Phillips Petroleum or Columbia Chemical; used as received.</li> <li>(2) distilled.</li> <li>ESTIMATED ERROR: temp. ± 1.5°C soly. 8 g(1)/10⁶ g(2) (standard deviation of mean)</li> <li>REFERENCES:</li> </ul>

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Polak, J.; Lu, B.CY.
(2) Water; H ₂ O; [7732-18-5]	Can. J. Chem. <u>1973</u> , 51, 4018-23.
•	
VARIABLES:	PREPARED BY:
Temperature: 0-25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	-l
	hylbenzene in water ·
	1)/100 g sln 10 ⁴ x ₁ (compiler) (compiler)
0(a) 197(c)	0.0197 3.34
25 (b) 177 (c)	0.0177 3.00
Solubility of wa	ter in ethylbenzene
t/°C mg(2)/kg(1) g	$\frac{10^3 x_2}{(\text{compiler})}$
0(a) 178(d)	0.0178 1.05
25 (b) 442 (e)	0.0442 2.60
AUXILIAR	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.	<pre>(1) Phillips Petroleum Co.; pure grade reagent (99+%); shaken three times with distilled water. (2) distilled. (2) distilled. (3) distilled. (4) distilled. (2) distilled. (2) distilled. (2) distilled. (3) distilled. (4) distilled. (2) distilled. (3) distilled. (4) distilled. (5) distilled. (6) distilled. (6) distilled. (7) distilled. (7)</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
	OROTAL MERSOREMIS.
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Brown, R.L.; Wasik, S.P.
(2) Water; H ₂ O; [7732-18-5]	J. Res. Natl. Bur. Stds. A. <u>1974</u> , 78, 453-60.
VARIABLES:	PREPARED BY:
Temperature: 4.5-20.1°C	G.T. Hefter
EXPERIMENTAL VALUES:	
Solubility of Eth	ylbenzene in Water
<u>t/°C</u> <u>g(l)/100 g sl</u>	$n^{a}$ $10^{5} x_{1}$ (compiler)
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	
7.1 0.0186 + 0.00	06 3 16
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	04 3.18
12.1 $0.0183 \pm 0.00$	04 3.11
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	05 3.06 05 3.12
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3.12
^D Typographical error in original pub decimal place.	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The appa- ratus and the method of obtaining the partition coefficients are described in detail in the paper. Basically, the hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing	<ol> <li>99.99 mole per cent purity; source and methods of purifi- cation not specified.</li> <li>Distilled.</li> </ol>
about 45 cm of water. The vapor was	ESTIMATED EDDOD.
subsequently analysed by gas chroma- tography using He as the carrier.	ESTIMATED ERROR:
Possible sources of error are dis- Cussed in detail although the source	Temperature: ±0.01°C
of vapor pressure data used to calcu-	Solubility: See Table above.
late solubilities are not given.	REFERENCES:

80	
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wa	ter at 25°C was reported to be
161.2 mg(1)/kg(2). The corresponding	g mass percent and mole fraction,
$x_1$ , calculated by the compilers are 0 2.734 x 10 ⁻⁵ .	0.01612 g(1)/100 g sln and
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	<ul> <li>(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.</li> <li>(2) distilled.</li> </ul>
	ESTIMATED ERROR: temp. ± 0.1°C soly. 0.9 mg(1)/kg(2) (the standard deviation of the mean for six replicates) REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4] (2) Water; H ₂ O; [7732-18-5]	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

# EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C and at system pressure was reported to be 131.0 mg(1)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 0.0131 g(1)/ 100 g sln and 2.22 x 10⁻⁵.

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de- tails are given in the paper.	<ul> <li>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>(2) distilled.</li> <li>ESTIMATED ERROR: temp. ± 1°C soly. ± 1.4 mg(1)/kg(2)</li> </ul>
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Korenman, I.M.; Aref'eva, R.P.	
(2) Water; H ₂ O; [7732-18-5]	Patent USSR, 553 524, 1977.04.05 C.A. <i>87</i> :87654.	
VARIABLES:	PREPARED BY:	
One temperature: 20°C	A. Maczynski	
- · •		
EXPERIMENTAL VALUES:		
The solubility of ethylbenzene in water at 20°C was reported to be 0.21 g(1) $L^{-1}$ (2). The corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are 0.021 g(1)/100 g sln and 3.6 x 10 ⁻⁵ . The assumption that 1 dm ³ sln = 1 kg sln was used in the calculation.		
	INFORMATION	
METHOD/APPARATUS/PROCEDURE: About 100-500 mL(2) was placed in a glass cylinder and 10-50 mg of an insoluble indicator was added and (1) was microburetted until	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.	
the indicator floated to form a colored thin layer on the cylinder wall 2-3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5-1.5 min.		
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES :	

	83		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Korenman, I.M.; Aref'eva, R.P.		
(2) Water; H ₂ O; [7732-18-5]	Zh. Prikl. Khim. <u>1978</u> , 51, 957-8.		
VARIABLES:	PREPARED BY:		
Temperature: 25°C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
The solubility of ethylbenzene in wate 0.18 g(l) $L^{-1}$ sln.	er at 25°C was reported to be		
The corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are 0.018 g(l)/100 g sln and 3.1 x 10 ⁻⁵ . The assumption that 1.00 L ⁻¹ = 1.00 kg sln was used in the calculation.			
AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
About 200-500 mL (2) was placed in a ground-joint glass cylinder and 20-50 mg of an insoluble indicator (dithizon, phenolphthalein, etc.) was added, and (1) was microburetted	(1) Not specified.		
	(2) Not specified.		
until the indicator floated to form a colored thin layer on the cylinder wall above the liquid layer. Blanks			
were made to determine the excess of (1).			
]	ESTIMATED ERROR:		
	Soly. 0.01 g(1) L ⁻¹ sln (std. dev. from 6 deter- minations).		
	REFERENCES:		
	1		

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COMPONENTS:
(1) Ethylbenzene; C8H10; [100-41-4]
(2) Water; H20; [7732-18-5]ORIGINAL MEASUREMENTS:
Krzyzanowska, T.; Szeliga, J.
Nafta (Katowice), 1978, 12, 413-7.VARIABLES:
One temperature: 25°CPREPARED BY:
M.C. Haulait-Pirson
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#### EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 131.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 0.0131 g(1)/100 g sln and 2.22 x  $10^{-5}$ .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.	
	ESTIMATED ERROR: soly. 3.4 mg(l)/kg(2) (standard deviation from 7-9 determinations). REFERENCES:	

COMPONENTS :		
	ORIGINAL MEASUREMENTS:	
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H.	
(2) Water; H ₂ O; [7732-18-5]	Chem. Lett. <u>1981</u> , 225-8.	
VARIABLES:	PREPARED BY:	
Temperature: 15-45°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:	l	
Solubility of et	nylbenzene in water	
t/°C g(l)/L	$\frac{g(1)/100 \text{ g sln}^{a}}{10^{4}x_{1}^{a}}$	
15 0.176 ± 0.009	0.0176 2.99	
	0.0182 3.09	
35 0.194 ± 0.006	0.0195 3.31	
45 0.215 ± 0.004	0.0217 3.69	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
METHOD/APPARATUS/PROCEDURE: The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel respectively. The solute vapor, gen- erated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/ min. Solubility equilibria were	SOURCE AND PURITY OF MATERIALS: (1) analytical reagent grade used as purchased. (2) redistilled.	
METHOD/APPARATUS/PROCEDURE: The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel respectively. The solute vapor, gen- erated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/ min. Solubility equilibria were attained within 5 min. Then portions	SOURCE AND PURITY OF MATERIALS: (1) analytical reagent grade used as purchased. (2) redistilled.	
METHOD/APPARATUS/PROCEDURE: The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel respectively. The solute vapor, gen- erated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/ min. Solubility equilibria were	SOURCE AND PURITY OF MATERIALS: (1) analytical reagent grade used as purchased. (2) redistilled.	

COMPONENTS :		ORIGINAL MEASUREMENTS:	
	NIS:       ORIGINAL MEASUREMENTS:         Sanemasa, I.; Araki, M.;         Iter; H ₂ O; [7732-18-5]         Deguchi, T.; Nagai, H.         Bull. Chem. Soc. Jpn. <u>1982</u> , 55, 105		н.
VARIABLES:	<u> </u>	PREPARED BY:	
Temperature: 1	5-45°C	G.T. Hefter	
EXPERIMENTAL VALU	ES:		
The solubility of ethylbenzene in water			
<i>t</i> /°C	10 ³ mol(1)/dm ³ sln	g(1)/100 g sln (compiler) ^a	$10^5 x_1$ (compiler) ^a
15 25 35 45	1.51 ± 0.08 1.59 ± 0.05 1.54 ± 0.05 1.83 ± 0.05	0.0160 0.0169 0.0176 0.0196	2.72 2.87 2.99 3.33
	emperature (ref 1).		
	AUXILIARY	INFORMATION	
earlier design described in d 100-200 cm ³ of liquid (1) wer but connected After thermal lished a recir was used to va to transport t containing (2) were withdrawn funnels. The (2) was then d into chlorofor spectrophotome	PROCEDURE: is similar to an (ref 2) and is etail in the paper. (2) and 10-20 cm ³ of e placed in separate thermostatted flasks. equilibrium was estab- culating stream of air porize liquid (1) and he vapor to the flask . Five 10 cm ³ aliquots into separatory concentration of (1) in etermined by extraction m followed by UV- etry. Standards for the etry were prepared by are liquid solutes.	Pure Chemical I purity 98.0%, u further purific	gent grade (Wako Ind. Ltd.), stated used without sation. b further details be of error not <u>1975</u> , 20, 97. aki, M.; ai, H.

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COMPONENTS: (1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. Bull. Chem. Soc. Jpn. <u>1984</u> , 57, 1539-44.
VARIABLES: One Temperature: 25°C	PREPARED BY: G.T. Hefter
EXPERIMENTAL VALUES: The solubility of ethylbenzene in wate 1.62 x 10 ⁻³ mol(1)/dm ³ sln. Assuming this corresponds to a solubility of 0. calculated by the compiler.	
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The apparatus used is described in detail in ref 1. The method involves the introduction of solute vapor(1) into liquid (2) by bubbling air through liquid (1) using a recirculat- ing pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analysed by solvent extraction - UV spectro-	<ul> <li>(1) Analytical reagent grade source and purity not stated, used without further purification.</li> <li>(2) Deionized and redistilled; no further details given.</li> </ul>
photometry.	ESTIMATED ERROR:
	Not specified.
	<pre>REFERENCES: 1. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62.</pre>

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Ethylbenzene; C₈H₁₀; [100-41-4] Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. (2) Water, H₂O; [7732-18-5] A. I. Ch. E. J. <u>1985</u>, 31, 376-84. VARIABLES: PREPARED BY: Temperature: 311-568 K G.T. Hefter Pressure: 0.01-10.7 MPa EXPERIMENTAL VALUES: Solubility of ethylbenzene in water  $10^4 x_1$ g(1)/100 g sln T/K p /MPa (compiler) _ a 0.019 311.5 0.32 0.86 0.051 367.6 0.111 2.19 0.129 423.4 0.627 6.0 0.35 479.5 2.32 1.88 536.1 6.50 32.5 37.5 2.17 552.8 8.59 a Not specified.

(continued)

AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.	purity ≥ 99.9 mol %, checked
	<pre>ESTIMATED ERROR: soly. ± 5%, relative precision of replicate analyses. temp. not stated. press. ± 1%; type of error not stated. REFERENCES: 1. Tsonopoulos, C.; Wilson, G.M. A. I. Ch. E. J. <u>1983</u>, 29, 990-9.</pre>

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 (1) Ethylbenzene; C<sub>8</sub>H<sub>10</sub>; [100-41-4]
 (2) Water, H<sub>2</sub>O; [7732-18-5]
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(continued)

#### Solubility of water in ethylbenzene

т/к	р /МРа	10 ² x ₂	g(2)/100 g sln (compiler)
310.9	0.0091 ^{<i>a</i>}	0.43	0.073
367.6	0.111	1.86	0.320
423.4	0.627	5.96	1.06
479.5	2.32	16.3	3.20
536.1	6.50	40.8	10.5
550.4	8.27	47.2	13.2
568.1 ^b	10.68 ^b	69.1 ^b	27.5

a Estimated by the authors from pure component data.b Three phase critical point.

The three phase critical point was reported to be 568.1  $\pm$  0.6 K, 10.68  $\pm$  0.04 MPa and  $x_1 = 5.83 \times 10^{-3}$  (3.34 g(1)/100 g sln, compiler).

The authors also report an equation providing a fit of their own and literature data over the range 273-568 K, viz.

 $\ln x_1 = -185.1695 + 7348.55/T + 26.34525 \ln T$  $\ln x_2 = -0.37215 - 4.4626 (T_r^{-1} - 1) - 0.38596 (1 - T_r)^{1/3}$  $- 2.59850 (1 - T_r)$ 

where  $T_r = T/568.1$ 

COMPONENTS:		ORIGINAL	MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [	100-41-4]	Brown	, R.L.; Wasik, S.P.
(2) Artificial seawater		J. Re 78, 4	s. Natl. Bur. Stds. A. <u>1974</u> , 53-60.
VARIABLES:		PREPAREI	D BY:
Temperature: 0-20°C Salinity: 34.42 g salts/kg	r el n	G.T.	Hefter and D.G. Shaw
EXPERIMENTAL VALUES:		· · · · ·	
Solubility of ethylbenzene in artificial seawater			
t∕°C g	(1)/100 g s	_1_a	$10^5$ (correction)
			$\frac{10^5 x_1 (\text{compiler})}{10^5 x_1 (\text{compiler})}$
	.0140 (0.00	-	2.44
	.0133 (0.00	-	2.31
	0.0129 (0.00		2.25
	.0125 (0.00		2.18
20.04 0	.0122 (0.00	003)	2.12
	AUXILIARY	INFORMAT	10N
METHOD/APPARATUS/PROCEDURE:			
			AND PURITY OF MATERIALS:
Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of ob- taining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 L of water. The vapor was		(2)	99.99 mole per cent purity; source and methods of purifi- cation not specified. Prepared according to ref 1. Purity not specified.
about 45 L of water. The v subsequently analysed by ga	apor was s chromato-	1	ED ERROR:
graphy using He as the carr	ier.	Temper	rature: ±0.01 K
Possible sources of error a cussed in detail although t	re dis- he source	Solub:	ility: see Table above
of vapor pressure data used culate solubilities are not	to cal-	Fle Pre	CES: erdrup, H.U.; Johnson, M.W.; eming, R.H.; The Oceans, <u>1942</u> , entice-Hall, Englewood Cliffs, v Jersey, p186.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 4-Vinyl-1-cyclohexene; C₈H₁₂; [100-40-3]</pre> (2) Water; H ₂ O; [7732-18-5]	McAuliffe, C. J. Phys. Chem. <u>1966</u> , 70, 1267-75.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of 4-vinyl-1-cyclohexe to be 50 g(1)/10 ⁶ g(2). The corresponding mass percent and mo by the compilers are 0.005 g(1)/100 c	ble fraction, $x_1$ , calculated
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS;
METHOD/APPARATUS/PROCEDURE: In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromato- graphed in conjunction with a flame- ionization detector.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 5 g(1)/10⁶ g(2) (standard deviation of mean) REFERENCES:</pre>

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COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Propenylcyclopentane; C₈H₁₄; [5623-78-9]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
One temperature: 30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of water in 1-propenyl reported to be 0.0383 g(2)/100 g sln. mole fraction, $x_2$ , calculated by the	The corresponding value
	INFORMATION
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hr with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: (1) 1-Octyne; C₈H₁₄; [629-05-0] McAuliffe, C. J. Phys. Chem. 1966, 70, 1267-75. (2) Water; H₂O; [7732-18-5] VARIABLES: PREPARED BY: A. Maczynski, Z. Maczynska, and One temperature: 25°C A. Szafranski **EXPERIMENTAL VALUES:** The solubility of 1-octyne in water at 25°C was reported to be 24  $q(1)/10^6 q(2)$ . The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compilers are 0.0024 g(1)/100 g sln and 4.4  $\dot{x}$  10⁻⁶. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: In a 250-mL bottle, 10-20 mL of (1) (1) Phillips Petroleum or was vigorously shaken for 1 hr, or Columbia Chemical; used magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to as received. (2) distilled. allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame- ESTIMATED ERROR: ionization detector. temp. ± 1.5°C soly. 0.8  $g(1)/10^6$  g(2)(standard deviation of mean) **REFERENCES:** 

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,1,3-Trimethylcyclopentane; C ₈ H ₁₆ ; [4516-69-2]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	L
The solubility of 1,1,3-trimethylcycl	opentane in water at 25°C and at
system pressure was reported to be 3.	
The corresponding mass percent and mo compiler are $3.73 \times 10^{-4} \text{ g(1)/100 g s}$	
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at	<ol> <li>Phillips Petroleum Company;</li> </ol>
laboratory temperatures by use of screw-cap test tubes. The (1) phase	Chemical Samples Company or or Aldrich Chemical Company;
floated on top of the water and insured saturation of the (2) phase	99+8.
in 2 to 4 days. Analyses were car-	(2) Distilled.
ried out by GLC using a Hewlett- Packard model 5751 gas chromatograph	
with dual-flame ionization detectors. Many details are given in the paper.	
decurre are given in the paper,	
	ESTIMATED ERROR:
	Temp. ±l°C
	Soly. ±0.17 mg(1)/kg(2)
	REFERENCES :

<pre>COMPONENTS: (1) 1,1,3-Trimethylcyclopentane;</pre>	ORIGINAL MEASUREMENTS:
	Krzyzanowska, T.; Szeliga, J.
C ₈ H ₁₆ ; [4516-69-2]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1,1,3-trimethylcycl	opentape in water at 25°C was
reported to be 2.04 $mg(1)/kg(2)$ .	
	lo fraction a coloulated
The corresponding mass percent and mo by compiler are 2.04 $\times$ 10 ⁻⁴ g(1)/100	-
by compiler are 2.04 x 10 $g(1)/100$	g sin and $3.27 \times 10^{-1}$ .
Editor's Note: Based on the results	for this and other hydrocarbon-water
systems, uncertainity exists about wh	
independent of that of Price for the	
	same system (see previous page). n evaluated.
Consequently, this system has not bee	
Consequently, this system has not bee	
Consequently, this system has not bee	n evaluated.
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in	n evaluated. INFORMATION
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS;
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1)	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS; (1) not specified.
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS; (1) not specified.
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS; (1) not specified.
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by qlc. A	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS; (1) not specified.
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS; (1) not specified.
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame	<pre>n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.10 mg(1)/kg(2) (standard</pre>
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.10 mg(1)/kg(2) (standard deviation from 7-9 determinations).
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	<pre>n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.10 mg(1)/kg(2) (standard</pre>
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.10 mg(1)/kg(2) (standard deviation from 7-9 determinations).
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.10 mg(1)/kg(2) (standard deviation from 7-9 determinations).
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.10 mg(1)/kg(2) (standard deviation from 7-9 determinations).
Consequently, this system has not bee AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	n evaluated. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.10 mg(1)/kg(2) (standard deviation from 7-9 determinations).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Isopropylcyclopentane; C₈H₁₆; [3875-51-2]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of water in	isopropylcyclopentane
<u>t/°C</u> <u>g(2)/1</u>	$\frac{10^4 x_2}{2} \text{ (compiler)}$
10 0.	0059 3.68
20 0.	0102 6.35
30 0.	9.90
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(1) not specified.
for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(2) not specified.
	ESTIMATED ERROR:
1	not specified.
	not protition.
	not specifica.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Propylcyclopentane; C₈H₁₆; [2040-96-2]</pre>	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
(2) (1202) 120, [1002 -0 0]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of propylcyclopentane	in water at 25°C and at
system pressure was reported to be 2.	
corresponding mass percent and mole f	raction, $x_1$ , calculated
by the compiler are 2.04 x $10^{-4}$ g(l)/	100 g sln and $3.27 \times 10^{-1}$ .
1	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at	(1) Phillips Petroleum Company;
laboratory temperatures by use of screw-cap test tubes. The (1)	Chemical Samples Company or Aldrich Chemical Company;
phase floated on top of the water and insured saturation of the (2)	99+%.
phase in 2 to 4 days. Analyses	(2) distilled.
were carried out by GLC using a Hewlett-Packard model 5751 gas	
chromatograph with dual-flame	
ionization detectors. Many details are given in the paper.	
	ESTIMATED ERROR:
	temp. ± 1°C soly. ± 0.10 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Propylcyclopentane; C₈^H₁₆;</li> </ol>	Krzyzanowska, T.; Szeliga, J.
[2040-96-2]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	

The solubility of propylcyclopentane in water at 25°C was reported to be 1.77 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 1.77 x  $10^{-4}$  g(1)/100 g sln and 2.84 x  $10^{-7}$ .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

#### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	<pre>(1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.07 mg(1)/kg(2) (standard deviation from 7-9 determinations).</pre>
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) cis-1,2-Dimethylcyclohexane; C₈H₁₆; [2207-01-4] (2) Water; H₂O; [7732-18-5]</pre>	McAuliffe, C. J. Phys. Chem. <u>1966</u> , 70, 1267-75.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES:	♣,,,,,,,,,,,,,_,_,
The solubility of cis-1,2-dimethylcyd reported to be 6.0 g(1)/10 ⁶ g(2). The corresponding mass percent and mo by the compilers are 0.00060 g(1)/100	ble fraction, $x_1$ , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromato-	<ul> <li>(1) Phillips Petroleum or Columbia Chemical; used as received.</li> <li>(2) distilled.</li> </ul>
graphed in conjunction with a flame-	ESTIMATED ERROR:
ionization detector.	temp. $\pm$ 1.5°C soly. 0.8 g(1)/10 ⁶ g(2) (standard deviation of mean)
	REFERENCES :

COMPONENTS :		ORIGINAL MEASUREMENTS:		
(1) 1,4-Dimethyl [589-90-21	<pre>(1) 1,4-Dimethylcyclohexane; C₈H₁₆; [589-90-2]</pre>		Guseva, A.N.; Parnov, E.I.	
(2) Water; H ₂ O; [7732-18-5]		Vestn. Mosk. Univ. Khim. <u>1964</u> , 19, 77-8.		
VARIABLES:		PREPARED BY:		
Temperature: 57-	240°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:		]		
Solu	bility of 1,4-dimethy	ylcyclohexane in water		
t/°C	g(l)/100 g(2)	g(1)/100 g sln (compiler)	10 ⁴ x1 (compiler)	
57	0.0017	0.0017	0.027	
105	0.0056	0.0056	0.090	
165	0.0263	0.0263	0.422	
240	0.257	0.257	4.120	
<del>-</del>				
METHOD/APPARATUS/PRO		INFORMATION SOURCE AND PURITY OF MATE		
		1	KIALS;	
made in sealed g	1. No more details	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>		
		ESTIMATED ERROR:		
		not specified.		
		REFERENCES: 1. Guseva, A.N.; Pa Vestn. Mosk. Uni 18, 76.		

COMPONENTS:       ORIGINAL MEASUREMENTS:         (1) 1,4-trans-Dimethylcyclohexane;       Price, L.C. $C_8^{H_16}$ ; [2207-04-7]       Am. Assoc. Petrol. Geol. Bull.         (2) Water; H ₂ O; [7732-18-5]       1976, 60, 213-44.	
C ₈ H ₁₆ ; [2207-04-7] Am. Assoc. Petrol. Geol. Bull.	
Am. Assoc. Petrol. Geol. Bull.	
(2) Water; $H_2O$ ; [7732-18-5] <u>1976</u> , 60, 213-44.	
VARIABLES: PREPARED BY:	
One temperature: 25°C M.C. Haulait-Pirson	
•	
EXPERIMENTAL VALUES:	
The solubility of 1,4-trans-dimethylcyclohexane in water at 25°C	
and at system pressure was reported to be $3.84 \text{ mg}(1)/\text{kg}(2)$ . The	
corresponding mass percent and mole fraction, $x_1$ , calculated	
by the compiler are 3.84 x $10^{-4}$ g(1)/100 g sln and 6.16 x $10^{-7}$ .	
	ĺ
AUXILIARY INFORMATION	
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The solubility was determined at (1) Phillips Petroleum Company;	
METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of Chemical Samples Company or	
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.	
METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company;	
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.	
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.	
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.	
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.SOURCE AND PURITY OF MATERIALS:(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.(2) distilled.	
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.SOURCE AND PURITY OF MATERIALS:(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.(2) distilled.(2) distilled.(2) distilled.(2) distilled.	
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.SOURCE AND PURITY OF MATERIALS:(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.(2) distilled.	
<pre>METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper. ESTIMATED ERROR: temp. ± l°C soly. ± 0.17 mg(1)/kg(2)</pre>	
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.(2) distilled.(2) distilled.ESTIMATED ERROR: temp. ± 1°C	
<pre>METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper. ESTIMATED ERROR: temp. ± l°C soly. ± 0.17 mg(1)/kg(2)</pre>	
<pre>METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper. ESTIMATED ERROR: temp. ± l°C soly. ± 0.17 mg(1)/kg(2)</pre>	
<pre>METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper. ESTIMATED ERROR: temp. ± l°C soly. ± 0.17 mg(1)/kg(2)</pre>	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>1,4-Dimethylcyclohexane; C₈H₁₆;</li> </ol>	Krzyzanowska, T.; Szeliga, J.
[589-90-2]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	I
EXPERIMENTAL VALUES:	

The solubility of 1,4-dimethylcyclohexane in water at 25°C was reported to be 3.84 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 3.84 x  $10^{-4}$  g(1)/100 g sln and 6.16 x  $10^{-7}$ .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

#### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
LIGINOD/ALLARATOS/LKOCEDURE.	SOURCE AND FURITI OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>
ograph equipped with a 100-150 mesh	
	FSTIMATED FRROR.
Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	ESTIMATED ERROR: soly. 0.12 mg(1)/kg(2) (standard deviation from 7-9 determinations).
ionization detector was used. Sat- urated solutions of heptane in (2)	soly. 0.12 mg(l)/kg(2) (standard

COMPONENTS :	EVALUATOR:
<pre>(1) Ethylcyclohexane; C₈H₁₆; [1678-91-7] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. May 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the ethylcyclohexane (1) - water (2) system have been reported in the publications listed in Table 1.

### TABLE 1: Quantitative Solubility Studies of theEthylcyclohexane (1) - Water (2) System

Reference	T/K	Solubility	Method
Guseva and Parnov (ref 1)	352-486	(1) in (2)	unspecified ^a
Heidman <i>et al</i> . (ref 2)	311-561	mutual	GLC, Karl Fischer

a Probably using the synthetic method.

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system is in two parts.

#### 1. SOLUBILITY OF ETHYLCYCLOHEXANE (1) IN WATER (2)

This system almost certainly exhibits type III phase behaviour (see introductory material at the beginning of this volume). The phase diagram is similar to that of ethylbenzene and water.

The solubility of ethylcyclohexane in water at elevated temperatures and system pressures along the three phase equilibrium line have been investigated by Guseva and Parnov (ref 1) and Heidman *et al.* (ref 2). Their results are summarized in Table 2 and plotted in Figure 1. The agreement is very poor. However, it may be noted (ref 1) that the values reported by Guseva and Parnov at higher temperatures approach those of cyclohexane which is unreasonable. It may also be noted that the data of Guseva and Parnov often differ markedly from Recommended values in other systems. The data of Heidman *et al.* are thus considered Tentative.

Heidman *et al*. report a three phase critical end point at 561.4  $\pm$  0.6 K, 9.93  $\pm$  0.04 MPa and  $x_1 = 3.35 \times 10^{-3}$  (2.05 g(1)/100g sln, Evaluator).

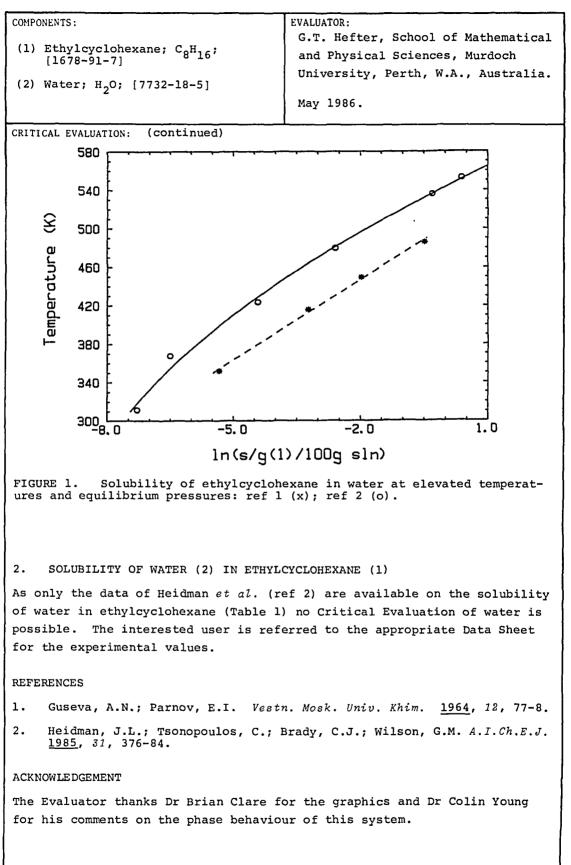
COMPONENTS:	EVALUATOR:
<pre>(1) Ethylcyclohexane; C₈H₁₆; [1678-91-7]</pre> (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
6	May 1986.

CRITICAL EVALUATION: (continued)

# TABLE 2: Tentative Solubility Values for Ethylcyclohexane (1) inWater (2) at the Three-Phase Equilibrium Pressure

T/K		ity values	1
	Reported values ^a	"Best" valu	es ^b
	10 ² g(1)/100g sln	10 ² g(1)/100g sln	10 ⁴ x1
313	0.066 (ref 2)	0.07	0.01
323	0.074 (ref 2)	0.07	0.011
333	0.086 (ref 2)	0.07	0.014
343	0.10 (ref 2)	0.10	0.016
353	0.5 (ref 1), 0.13 (ref 2)	0.13	0.020
363	0.8 (ref 1), 0.16 (ref 2)	0.16	0.026
373	1.3 (ref 1), 0.21 (ref 2)	0.21	0.034
393	2.2 (ref 1), 0.55 (ref 2)	0.55	0.088
413	3.7 (ref 1), 0.95 (ref 2)	0.95	0.15
433	6.5 (ref 1), 1.6 (ref 2)	1.6	0.26
453	16.0 (ref 1), 2.8 (ref 2)	2.8	0.45
473	27.0 (ref 1), 5.5 (ref 2)	5.5	0.9
493	16 (ref 2)	16	2.2
513	34 (ref 2)	34	5.2
533	65 (ref 2)	65	10.4
553	150 (ref 2)	150	24.0

a All data obtained by graphical or algebraic interpolation by the Evaluator of the authors' original data.
b Rounded values from ref 2; data from ref 1 not included in "Best" values, see text.



MPONENTS :	ORI	GINAL MEASUREME	INTS:	
<pre>(1) Ethylcyclohexane; C₈H₁₆; [1678-91-7] (2) Water; H₂0; [7732-18-5]</pre>		Guseva, A.N.; Parnov, E.I.		
		Vestn. Mosk. Univ. Khim. <u>1964</u> , 19, 77-8.		
RIABLES:	PRE	PREPARED BY:		
Cemperature: 79-213°C	м.	C. Haulait-P	irson	
PERIMENTAL VALUES:				
Solubility of a	ethylcyclob	exane in wat	er	_
t/°C g(1)/100 g	g (2)	g(l)/l00 g (compiler	sln <u>) (c</u> e	10 ⁴ x ₁ ompiler)
79 0.004	8	0.0048		0.077
142.5 0.039		0.0398		0.639
176 0.138		0.138		2.22
213 0.66		0.62		9.96
A	AUXILIARY INFO	RMATION		
	SOU	RCE AND PURITY		
THOD/APPARATUS/PROCEDURE:	ere (]			
THOD/APPARATUS/PROCEDURE: Presumably the measurements we hade in sealed glass tubes, a reported in ref 1. No more do	ere (]	RCE AND PURITY	ied.	;
THOD/APPARATUS/PROCEDURE: Presumably the measurements we hade in sealed glass tubes, a reported in ref 1. No more do	ere (]	RCE AND PURITY ) not specif	ied.	
THOD/APPARATUS/PROCEDURE: Presumably the measurements we hade in sealed glass tubes, a reported in ref 1. No more do	ere (1 s etails (2	RCE AND PURITY ) not specif ) not specif	ied.	3
THOD/APPARATUS/PROCEDURE: Presumably the measurements we hade in sealed glass tubes, a reported in ref 1. No more do	ere (] s etails (2 EST	RCE AND PURITY ) not specif	ied.	2
A THOD/APPARATUS/PROCEDURE: Presumably the measurements we hade in sealed glass tubes, a reported in ref 1. No more do vere reported in the paper.	ere (1 s etails (2 EST nc	RCE AND PURITY ) not specif ) not specif IMATED ERROR: t specified. ERENCES: Guseva, A.	ied.	, E.I.

			ORIGINAL MEASUREMENTS:		
1) Ethylcyclohexane; C ₈ H ₁₆ ; [1678-91-7]			Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M.		
-	Water, H ₂ O; [7732-18-5]		. E. J. <u>1985</u> , 31, 376-84.		
ARIABLES: Cemperature: 311-561 K Pressure: 0.01-9.9 MPa			PREPARED BY: G.T. Hefter		
PERIMENTAL VALU	ES:				
	Solubility of	ethylcyclohexan	e in water		
<i>T</i> / K	р /МРа	10 ⁴ x ₁	10 ² g(1)/100 g sln (compiler)		
311.5	_ a	0.011	0.068		
367.6	0.117	0.024	0.15		
423.4	0.647	0.20	1.2		
479.5	2.36	1.21	7.5		
536.1	6.69	11.8	73		
552.8	8.83	23.7	146		
a Not spec	ified.				
a Not spec	ified.		(continued)		
a Not spec		XILIARY INFORMATION			
ETHOD/APPARATUS, xperimental p hat used in r ere determine nd water by F ritical point ynthetic meth tion. This a	AU PROCEDURE: procedure was simi ref. 1. Hydrocarb red by gas chromato carl Fischer titra	SOURCE AND lar to (1) Aldr ons puri- graphy by g tion. by the (2) Dist bserv- edure			

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 Ethylcyclohexane, C<sub>8</sub>H<sub>16</sub>; [1678-91-7]
 Water, H<sub>2</sub>O; [7732-18-5]
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(continued)

Solubility of water in ethylcyclohexane

T/K	р /МРа	10 ² x ₂	g(2)/100 g sln (compiler)
310.9	0.0099 ^a	0.081	0.0130
367.6	0.117	0.65	0.104
423.4	0.647	3.0	0.48
479.5	2.36	10.7	1.89
536.1	6.69	29.0	6.15
552.8	8.83	41.4	10.2
561.4 ^b	9.93 ^b	60.3 ^b	19.6

a Estimated by the authors from pure component data.

b Three phase critical point.

The three phase critical point was reported to be 561.4  $\pm$  0.6 K, 9.93  $\pm$  0.04 MPa and  $x_1 = 3.35 \times 10^{-3}$  (1.05 g(1)/100 g sln, compiler).

The authors also report an equation which fits their own and related literature data over the range 273-561 K, viz.

 $\ln x_1 = -334.2468 + 14105.21/T + 47.93102 \ln T$  $\ln x_2 = -0.50980 - 7.4603 (T_r^{-1} - 1) - 0.67885 (1 - T_r)^{1/3}$  $+ 0.44796 (1 - T_r)$ 

where  $T_p = T/561.4$ 

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) $Cycloogtape: C H : [292-64-8]$	McAuliffe, C.
(1) Cyclooctane; $C_{8}H_{16}$ ; [292-64-8]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
(2) Water; H ₂ O; [7732-18-5]	2. Frigs. Chem. <u>1900</u> , 707 1207 73.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
-	
EXPERIMENTAL VALUES:	
The solubility of cyclooctane in wate	r at 25°C was reported to
be 7.9 mg (1)/kg sln.	
The corresponding mole fraction, $x_1$ ,	calculated by the compiler,
is $1.27 \times 10^{-6}$ .	
The same value is also reported in re	£ 1.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250 mL glass bottle, 10-20 mL	(1) Phillips Petroleum Co.; 99+%
of (1) was vigorously shaken for 1 hr or magnetically stirred for	purity; used as received.
1 day, with 200 mL of (2) at 25°C.	(2) distilled.
In the case of shaking, the solution was allowed to stand for 2 days to	
permit separation of small (1) drop- lets. Absence of emulsion was	
checked microscopically. A 50 µL sample of the (1) saturated water	
was withdrawn with a Hamilton Syringe and injected into the frac-	
tionator of the gas chromatograph.	ESTIMATED ERROR: temp. ± 1.5°C
A hydrogen-flame ionization detector was used. Many details are given in	soly. 1.8 mg (1)/kg sln (standard deviation from mean)
the paper.	
	REFERENCES: 1. McAuliffe, C. Am. Chem. Soc.
	Div. Petrol. Chem. <u>1964</u> , 9,
	275.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Octene; C ₈ H ₁₆ ; [111-66-0]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of 1-octene in water a to be 2.7 g(1)/10 ⁶ g(2). The corresponding mass percent and mo by the compilers are 0.00027 g(1)/100	ble fraction, $x_1$ , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromato- graphed in conjunction with a flame- ionization detector.	<pre>(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 0.2 g(1)/10⁶ g(2) (standard deviation of mean) REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) l-Octene; C ₈ H ₁₆ ; [111-66-0] (2) Water; H ₂ 0 [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. J. Chem. Eng. Data <u>1972</u> , 17, 328-9
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson, G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of 1-octene in wat	er was reported to be 1.979 $\times$ 10 ⁻⁴

The solubility of 1-octene in water was reported to be 1.979 × 10 ⁻¹ mol L⁻¹ at 25°C.^{*a*} Assuming a solution density of 1.00 g mL⁻¹ the corresponding mass percent and mole fraction  $(x_1)$  solubilities calculated by the compilers are respectively, 0.00222 g(1)/100 g sln and 3.63 x 10⁻⁶.

Solubility data are also presented as a function of temperature in various salt solutions.

^{*a*} It should be noted that although the authors state that the solubility refers to "water" the context in the paper is ambiguous and the data were probably obtained in 0.001 mol L⁻¹ HNO₂ solution.

AUXILIARY	INFORMATION
ETHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted	<pre>(1) Matheson, Coleman and Bell; 99%</pre>
glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures.	(2) Not specified
	ESTIMATED ERROR:
	Temp. ± 0.05K Soly. not specified.
	REFERENCES:

	11
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Octene; C ₈ H ₁₆ ; [111-67-1]	Natarajan, G.S.; Venkatachalam, K.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 328-9.
VARIABLES :	
	PREPARED BY:
Temperature: 15-25°C	M.C. Haulait-Pirson, G.T. Hefter
EXPERIMENTAL VALUES:	
Solubility of 2-octene in 0.001 mol/L	HNO3 solution.
t/°C $10^4 \text{ mol/L sln}^a$ 10	$\begin{array}{llllllllllllllllllllllllllllllllllll$
15 2.92 ± 0.14	3.3 5.3
20 2.51 ± 0.16	2.8 4.5
25 2.16 ± 0.15	2.4 3.9
the low concentration of the added act solubility to differ markedly from the solubility data are given in the paper	at in pure water. Further
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures.	<ol> <li>Prepared by dehydration of 2-octanol and then washed, dried and fractionated. Purity (no specification) was determined by chromatography.</li> <li>Not specified.</li> </ol>
	ESTIMATED ERROR:
	Temp. ± 0.05 K Soly. see table above.
	REFERENCES :

COMPONENTS :	EVALUATOR:
<pre>(1) 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch
(2) Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia.
	January 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,2,4-trimethylpentane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2,2,4-Trimethylpentane (1) - Water (2) System

Reference	T/K	Solubility	Method
Berkengeim (ref l)	273-313	(2) in (1)	Karl Fischer
Baker (ref 2)	unspecified	(1) in (2)	radiotracer
Englin $et \ al.$ (ref 3)	273-323	(2) in (1)	analytical
McAuliffe (ref 4)	298	(l) in (2)	GLC
Polak and Lu (ref 5)	273,298	mutual	GLC, Karl Fischer
Budantseva <i>et al</i> . (ref 6)	293	mutual	unspecified
Price (ref 7)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 8)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediatley following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. THE SOLUBILITY OF 2,2,4-TRIMETHYLPENTANE (1) IN WATER (2)

Very few data are available for the solubility of 2,2,4-trimethylpentane in water making critical evaluation difficult. The datum of Baker (ref 2) is rejected as the temperature was not specified. All other reported values are collected in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 8) which does not appear to be independent of that of Price (ref 7) and has therefore been excluded from consideration.

At 298K where comparisons are possible, the values of McAuliffe (ref 4) and Polak and Lu (ref 5) are in reasonable agreement. The value reported by Price (ref 7) is much lower. Although Price's data for many hydrocarbons in water are normally reliable, many of his values for the higher hydrocarbons are lower than other studies. However, in the absence of confirmatory studies it is not reasonable to reject Price's value at this stage. However, it has not been included in the calculation of the "Best" values at 298K.

At other temperatures the "Best" values should be regarded with caution in the absence of confirmatory studies. (continued next page)

COMPONENTS :	EVALUATOR:
<pre>(1) 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch
(2) Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia. January 1986.

CRITICAL EVALUATION: (continued)

### TABLE 2: Tentative Values of the Solubility of2,2,4-Trimethylpentane(1) in Water(2)

T/K	Solubility values		
ſ	Reported values	"Best" value	
ļ	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln	10 ⁷ x ₁
273	2.46 (ref 5)	2.5	3.9
293	2 (ref 6)	2	3
298	2.44 (ref 4), 2.05 (ref 5) 1.14 (ref 7)	2.2 ± 0.2 ^b	3.5 ^b

α Obtained by averaging where appropriate; σ_n has no statistical significance.
 b Average of data from ref 4 and 5 only, see text.

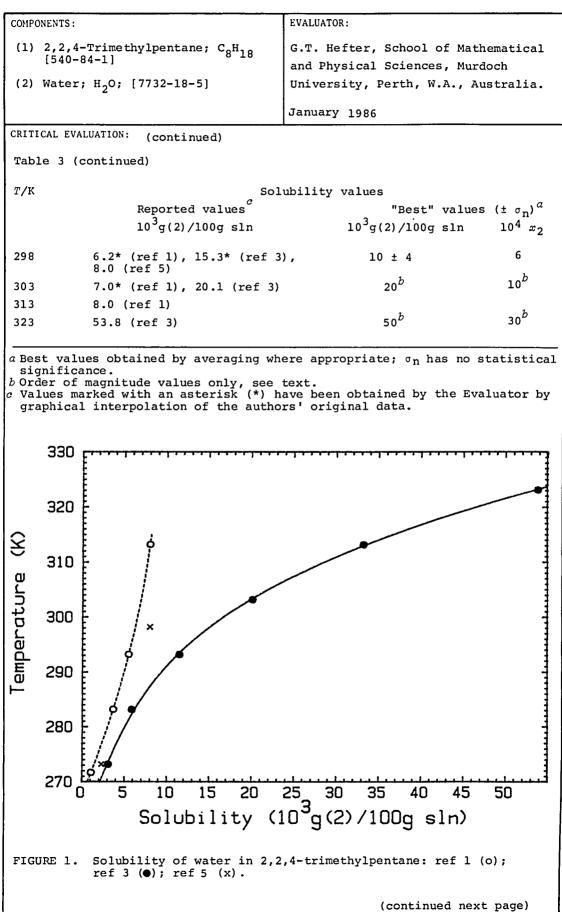
2. SOLUBILITY OF WATER (2) IN 2,2,4-TRIMETHYLPENTANE (1)

The various reported values of the solubility of water in 2,2,4-trimethylpentane are collected in Table 3 and plotted in Figure 1.

The data are generally in poor agreement and the averaged "Best" values must be regarded with caution pending further studies. Generally, for many other systems investigated by these authors, the data of Englin *et al*. (ref 3) are reliable at T < 300K but are too high at higher temperatures. Application of the van't Hoff equation to the data of Englin *et al*. and Bergengeim (ref 1) gives values of  $\Delta H_{\rm Sln} = 41.9$  and 20.1 kJ mol⁻¹ and  $\Delta C_{\rm p, Sln} = -100$  and -1950 J K⁻¹ mol⁻¹ respectively. Comparison of these data with other systems suggests that the values of Englin *et al*. are more realistic (although probably high at T > 300K). This system clearly warrants further investigation.

## TABLE 3: Tentative Values of the Solubility ofWater (2) in 2,2,4-Trimethylpentane (1)

T/K Solubility va		ty values	values	
	Reported values c	"Best" values (± d		
	10 ³ g(2)/100g sln	10 ³ g(2)/100g sln 10 ⁴	⁴ ^x 2	
273	1.7* (ref 1), 3.1 (ref 3), 2.3 (ref 5)	2.4 ± 0.6	1.5	
283	3.7 (ref 1), 5.9 (ref 3), 4.5* (ref 5)	4.7 ± 0.9	2.9	
293	5.5 (ref 1), 11.5 (ref 3), 6.5* (ref 5), 7.9 (ref 6)	8 ± 2	5	
		(Table 3 continued next p	page)	



COMP	DNENTS:	EVALUATOR:	
(1)	2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch	
(2)	Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia.	
		January 1986.	
CRIT	ICAL EVALUATION: (continued)		
REFI	ERENCES		
1.	Berkengeim, T.I. Zavod. Lab. 19	<u>941</u> , <i>10</i> , 592-4.	
2.	Baker, E.G. Geochim. Cosmochim. Acta <u>1960</u> , 19, 309-17.		
3.	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.		
4.	McAuliffe, C. J. Phys. Chem. <u>1966</u> , 70, 1267-75.		
5.	5. Polak, J.; Lu, B.CY. Can. J. Chem. <u>1973</u> , 51, 4018-23.		
6.	<ol> <li>Budantseva, L.A.; Lesteva, T.M.; Nemtsov, M.S. Zh. Fiz. Khim. <u>1976</u>, 50, 1344, Deposited doc. 1976, VINITI 437-76.</li> </ol>		
7.	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.		
8.	. Krzyzanowska, T.; Szeliga, J. <i>Nafta (Katowice)</i> <u>1978</u> , <i>34</i> , 413-7.		
ACKNOWLEDGEMENT			

The Evaluator thanks Dr Marie-Claire Haulait-Pirson for comments and Dr Brian Clare for the graphics and regression analyses.

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COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 2,2,4-Trimethylpentane; C₈H [540-84-1]</pre>	H ₁₈ ; Berkengeim, T.I.
(2) Water; H ₂ O; [7732-18-5]	Zavod. Lab. <u>1941</u> , 10, 592-4.
VARIABLES:	PREPARED BY:
Temperature: (-1.5) - 40°C	A. Maczynski
EXPERIMENTAL VALUES:	
Solubility of wate	er in 2,2,4-trimethylpentane
t/°C g(2)/1	$10^{4}x_{2}$ (compiler)
10 0 20 0	0.0011       0.697         .0037       2.35         .0055       3.49         .0080       5.07
ΔΤΤΧ	XILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	SOURCE AND FURTH OF PATERIALS;
The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	s (1) source not specified; CP reagent; d ²⁰ 0.6947; used as received.
	(2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	Baker, E.G.
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1960</u> , 19, 309-17.
VARIABLES:	PREPARED BY:
One temperature: not specified	M.C. Haulait-Pirson
one competatule, not specific	
EXPERIMENTAL VALUES:	<b>.</b>
The solubility of 2,2,4-trimethylpent	tane in water was reported
to be 0.0009 mL(1) $L^{-1}$ (2).	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The procedure is described in ref 1.	not specified.
	1
	ESTIMATED ERROR:
	not specified.
	not specifica.
	REFERENCES :
	1. Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints
	<u>1958</u> , 3, N°4, C61.

Components :	ORIGINAL MEASURE	EMENTS:	
<pre>(1) 2,2,4-Trimethylpentane;     [540-84-1]</pre>	C ₈ H ₁₈ ; Englin, B.A. V.M.; Pryar	; Plate, A.F.; Tugolu nishnikova, M.A.	ko
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhno 10, 42-6.	l. Topl. Masel <u>1965</u> ,	
VARIABLES:	PREPARED BY:	<u> </u>	
Temperature: 0-50°C	A. Maczynski	and M.C. Haulait-Pir	sor
EXPERIMENTAL VALUES:			
Solubility of wa	ter in 2,2,4-trimethyl	pentane	
<i>t</i> /°C	g(2)/100 g sln	$10^4 x_2$ (compile	r)
0	0.0031	1.97	
10	0.0059	3.74	
20	0.0115	7.29	
30	0.0201	12.74	
40	0.0332	21.02	
50	0.0538	34.03	

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURITY OF MATERIALS; (1) not specified. (2) not specified.
in (1) was evaluated.	ESTIMATED ERROR: not specified.
	REFERENCES :

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	McAuliffe, C.
	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2,2,4-trimethylpen to be 2.44 mg (1)/kg sln. The corresponding mole fraction, $x_1$ , is 3.85 x 10 ⁻⁷ . The same value is also reported in r	calculated by the compiler,
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) drop- lets. Absence of emulsion was checked microscopically. A 50 µL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the frac- tionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.	<ul> <li>(1) Phillips Petroleum Co.; 99+% purity; used as received.</li> <li>(2) distilled.</li> </ul>
	<pre>temp. ± 1.5°C soly. 0.12 mg (1)/kg sln (standard</pre>
	<ul> <li>REFERENCES:</li> <li>1. McAuliffe, C. Nature (London) 1963, 200, 1092.</li> <li>2. McAuliffe, C. Am. Chem. Soc., Div. Petrol. Chem. <u>1964</u>, 9, 275.</li> </ul>

ORIGINAL MEASUREMENTS:
Polak, J.; Lu, B.C-Y. Can. J. Chem. <u>1973</u> , 51, 4018-23.
PREPARED BY:
M.C. Haulait-Pirson
methylpentane in water
$s_1$ (compiler)
$\begin{array}{c} c \\ 3.88 \times 10^{-7} \\ c \\ 3.23 \times 10^{-7} \end{array}$
2,2,4-trimethylpentane sln $x_2$ (compiler)
$1.46 \times 10^{-4}$ 5.07 x 10 ⁻⁴
INFORMATION
<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled. (2) distilled. ESTIMATED ERROR: temp. a) ± 0.02°C; b) ± 0.01°C soly. c) ± 4%; d) ± 4.7%; e) ± 3.1% (mean) REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1]</pre>	Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S.	
(2) Water; H ₂ O; [7732-18-5]	Zh. Fiz. Khim. <u>1976</u> , 50, 1344. Deposited doc. <u>1976</u> , VINITI 437-76.	
VARIABLES:	PREPARED BY:	
One temperature: 20°C	A. Maczynski	
EXPERIMENTAL VALUES:		
The solubility of 2,2,4-trimethylpentane in water at 20°C was reported to be $x_1 = 3 \times 10^{-7}$ .		
The corresponding mass percent calculated by the compiler is about 2 x $10^{-4}$ g(1)/100 g sln.		
The solubility of water in 2,2,4-trimethylpentane at 20°C was reported to be $x_2 = 4.4 \times 10^{-4}$ .		
The corresponding mass percent value calculated by the compiler is 7.9 x $10^{-3}$ (2)/100 g sln.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Nothing specified in the paper.	(1) not specified.	
	(2) not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	
	L	
HWW 2-J		

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	Price, L.C. Am. Assoc. Petrol. Geol. Bull.
(2) Water; H ₂ O; [7732-18-5]	<u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2,2,4-trimethylpent and at system pressure was reported t corresponding mass percent and mole f by the compiler are 1.14 x 10 ⁻⁴ g(1)/	o be 1.14 mg(l)/kg(2). The raction, x ₁ , calculated
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<ol> <li>Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>distilled.</li> </ol>
	ESTIMATED ERROR:
	temp. ± 1°C soly. ± 0.02 mg(1)/kg(2)
	REFERENCES :

COMPON	ENTS:	ORIGINAL MEASUREMENTS:
(1)	2,2,4-Trimethylpentane; C ₈ H ₁₈ ;	Krzyzanowska, T.; Szeliga, J.
	[540-84-1]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2)	Water; H ₂ 0; [7732-18-5]	
VARIAB	LES:	PREPARED BY:
One	temperature: 25°C	M.C. Haulait-Pirson
EXPERI	MENTAL VALUES:	
to h	pe l.14 mg(l)/kg(2).	tane in water at 25°C was reported
	corresponding mass percent and m	—
by c	compiler are 1.14 x 10 ⁻⁴ g(1)/100	g sln and $1.80 \times 10$ '.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION				
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:			
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>			
(1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh				
Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	ESTIMATED ERROR: soly. 0.04 mg(1)/kg(2) (standard deviation from 7-9 determinations).			
	REFERENCES:			

COMPONENTS:	EVALUATOR:
<ol> <li>(1) 2,3,4-Trimethylpentane; C₈H₁₈; [565-75-3]</li> <li>(2) Water; H₂O; [7732-18-5]</li> </ol>	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	February 1986.

#### CRITICAL EVALUATION:

Quantitative solubility data for the 2,3,4-trimethylpentane (1) - water (2) system have been reported in the publications listed in Table 1.

### TABLE 1: Quantitative Solubility Studies of the2,3,4-Trimethylpentane (1) - Water (2) System

Reference	T/K	Solubility	Method
Polak and Lu (ref 1)	273,298	mutual	GLC, Karl Fischer
Price (ref 2)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. THE SOLUBILITY OF 2,3,4-TRIMETHYLPENTANE (1) IN WATER (2)

All the available data on the solubility of 2,3,4-trimethylpentane in water are collected in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 3) which does not appear to be independent of that of Price (ref 2) and has thus been excluded from consideration.

At 298K, the datum of Polak and Lu (ref 1) is much higher than that reported by Price (ref 2), as for many other hydrocarbon systems investigated by these authors. In the absence of other independent studies it is not possible to prefer either datum.

TABLE 2: Tentative Values of the Solubility of2,3,4-Trimethylpentane (1) in Water (2)

T/K	ty values	
	Reported values	"Best" values $(\pm \sigma_n)^a$
	10 ⁴ g(l)/100g sln	$10^4$ g(1)/100g sln 10 $x_1$
273	2.34 (ref 1)	2.3
298	2.30 (ref 1), 1.36 (ref 2)	1.8 ± 0.5

(continued next page)

COMPONENTS:	EVALUATOR:
<ol> <li>2,3,4-Trimethylpentane; C₈H₁₈; [565-75-3]</li> <li>Water; H₂O; [7732-18-5]</li> </ol>	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	February 1986.

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN 2,3,4-TRIMETHYLPENTANE (1)

As only one study of the solubility of water in 2,3,4-trimethylpentane has been reported (ref 1) no Critical Evaluation is possible. The interested user is referred to the appropriate Data Sheet for experimental values. However, it may be noted that the solubility of water in other hydrocarbons reported by Polak and Lu (ref 1) are normally reliable.

REFERENCES

1. Polak, J.; Lu, B.C-Y. Can. J. Chem. <u>1973</u>, 51, 4018-23.

- 2. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
- 3. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3,4-Trimethylpentane; C ₈ H ₁₈ ; [565-75-3]	Polak, J.; Lu, B.C-Y.
(2) Water; H ₂ O; [7732-18-5]	Can. J. Chem. <u>1973</u> , 51, 4018-23.
VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of 2,3,4-trin	methylpentane in water
t/°C mg(l)/kg	sln $x_1$ (compiler)
0 ^a 2.34 25 ^b 2.30	
Solubility of water in	
$\frac{t/^{\circ}C}{\frac{d}{d}}$ $\frac{mg(2)/kg}{d}$	<u>_</u>
0 ^a 20 ^d 25 ^b 74 ^e	$1.27 \times 10^{-4}$ 4.69 x 10 ⁻⁴
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titra- tion. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetical- ly for 24 hr or was kept in the	<ul> <li>SOURCE AND PURITY OF MATERIALS;</li> <li>(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water.</li> <li>(2) distilled.</li> </ul>
bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.	ESTIMATED ERROR: temp. a) ± 0.02°C; b) ± 0.01°C soly. c) ± 4%; d) ± 4.7%; e) ± 3.1% (mean) REFERENCES:

	12
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3,4-Trimethylpentane; C ₈ H ₁₈ ; [565-75-3]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2,3,4-trimethylpent at system pressure was reported to be corresponding mass percent and mole : by the compiler are 1.36 x 10 ⁻⁴ g(1),	e l.36 mg(l)/kg(2). The fraction, x _l , calculated _
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<ol> <li>Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>distilled.</li> </ol> ESTIMATED ERROR:
	temp. ± 1°C soly. ± 0.03 mg(1)/kg(2)
	2017. 7 0.02 mg(1)/KG(5)
	REFERENCES :

```
COMPONENTS:

(1) 2,3,4-Trimethylpentane; C<sub>8</sub>H<sub>18</sub>;

[565-75-3]

(2) Water; H<sub>2</sub>O; [7732-18-5]

VARIABLES:

One temperature: 25°C

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), <u>1978</u>, 12, 413-7.

PREPARED BY:

M.C. Haulait-Pirson
```

EXPERIMENTAL VALUES:

The solubility of 2,3,4-trimethylpentane in water at 25°C was reported to be 1.36 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 1.36 x  $10^{-4}$  g(1)/100 g sln and 2.14 x  $10^{-7}$ .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	<pre>(1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.05 mg(1)/kg(2) (standard deviation from 7-9 determinations).</pre>		
	REFERENCES :		

	13
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylhexane; C ₈ H ₁₈ ; [584-94-1]	Baker, E.G.
[584-94-1] (2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1960</u> , 19, 309-17.
VARIABLES:	PREPARED BY:
One temperature: not specified	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	······································
The solubility of 2,3-dimethylhexane 0.0002 mL(1)/L(2).	in water was reported to be
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The procedure is described in ref 1.	not specified.
	ESTIMATED ERROR: not specified. REFERENCES: 1. Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints 1958, 3, N°4, C61.

ENTS:		

COMPONENTS :	ORIGINAL MEASURI	EMENTS :	
(1) 2,4-Dimethylhexane; C ₈ H ₁₈ ; [589-43-5]		; Plate, A.F. nishnikova, N	
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhno 10, 42-6.	l. Topl. Mase	22 <u>1965</u> ,
VARIABLES:	PREPARED BY:		
Temperature: 10-30°C		A. Maczynski and M.C. Haulait-Pirs	
EXPERIMENTAL VALUES:	I		
Solubility of water	in 2,4-dimethylh		
t/°C g(2)	/100 g sln	$\frac{10^4 x_2}{2}$	(compiler)
10	0.0053	3.36	
	0.0098	6.21	
30	0.0180	11.41	
AUXILIA	RY INFORMATION		
	RY INFORMATION	TY OF MATERIALS:	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into	SOURCE AND PURI		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURI	ified.	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURI (1) not spec (2) not spec	ified. ified.	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURI (1) not spec	ified. ified.	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURI (1) not spec (2) not spec ESTIMATED ERROR	ified. ified.	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURI (1) not spec (2) not spec ESTIMATED ERROR not specifie	ified. ified.	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 3-Methylheptane; C ₈ H ₁₈ ; [589-81-1]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 3-methylheptane in pressure was reported to be 0.792 mg mass percent and mole fraction, $x_1$ , are 7.92 x $10^{-5}$ g(1)/100 g sln and 1.	(1)/kg(2). The corresponding calculated by the compiler
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<ol> <li>Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%.</li> <li>distilled.</li> </ol>
	ESTIMATED ERROR:
	temp. ± 1°C soly. ± 0.028 mg(1)/kg(2)
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 3-Methylheptane; C ₈ H ₁₈ ;	Krzyzanowska, T.; Szeliga, J.	
[589-81-1]	Nafta (Katowice), <u>1978</u> , 12, 413-7.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of 3-methylheptane	in water at 25°C was reported	
to be 0.792 mg(l)/kg(2).		
The corresponding mass percent and mole fraction, $x_1$ , calculated		
by compiler are 7.92 x $10^{-5}$ g(1)/100 g sln and 1.25 x $10^{-7}$ .		

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	<pre>(1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.04 mg(1)/kg(2) (standard deviation from 7-9 determinations). REFERENCES:</pre>	

COMPONENTS:	EVALUATOR:
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter [*] , School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	October 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the n-octane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the

Octa	ne (1) - Water	(2) System	
Reference	T/K	Solubility	Method
Fühner (ref 1)	289	(1) in (2)	titration
Black et al. (ref 2)	293	(2) in (1)	radiotracer
Baker (ref 3)	unspecified	(l) in (2)	radiotracer
Englin (ref 4)	283-303	(2) in (1)	analytical
McAuliffe (ref 5)	298	(1) in (2)	GLC
Nelson and De Ligny (ref 6)	278-318	(1) in (2)	GLC
Krasnoshchekova and Gubergrits (ref 9)	298	(1) in (2)	GLC
Polak and Lu (ref 10)	273,298	mutual	GLC, Karl Fischer
Budantseva <i>et al</i> . (ref 11)	293	mutual	unspecified
Price (ref 12)	298-423	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 13)	298	(1) in (2)	GLC
Skripka (ref 14)	498-538 ^a	(2) in (1)	unspecified
Jonsson $et \ al.$ (ref 15)	288-308	(1) in (2)	partition coefficient
Heidman <i>et al</i> . (ref 16)	311 <b>-</b> 539 ^{<i>a</i>}	mutual	synthetic

a High pressure data

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition critical phenomena have been investigated by Roof (ref 8). These are considered along with solubility data at high pressures in Section 3 below.

For convenience further discussion of this system will be in three parts.

1. THE SOLUBILITY OF OCTANE (1) IN WATER (2)

Agreement amongst the independent determinations of the solubility of octane in water is not particularly good and no data have been Recommended.

At 298K the value reported by Price (ref 11) is substantially lower than all other studies (ref 5,9,10,15) and has been rejected. At higher temp-(continued next page

*Section 3 was written with C.L. Young, Department of Physical Chemistry, University of Melbourne, Australia.

COMPONENTS:	EVALUATOR:
(2) Water: $H O: [7732-18-5]$	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	October 1986.

CRITICAL EVALUATION: (continued)

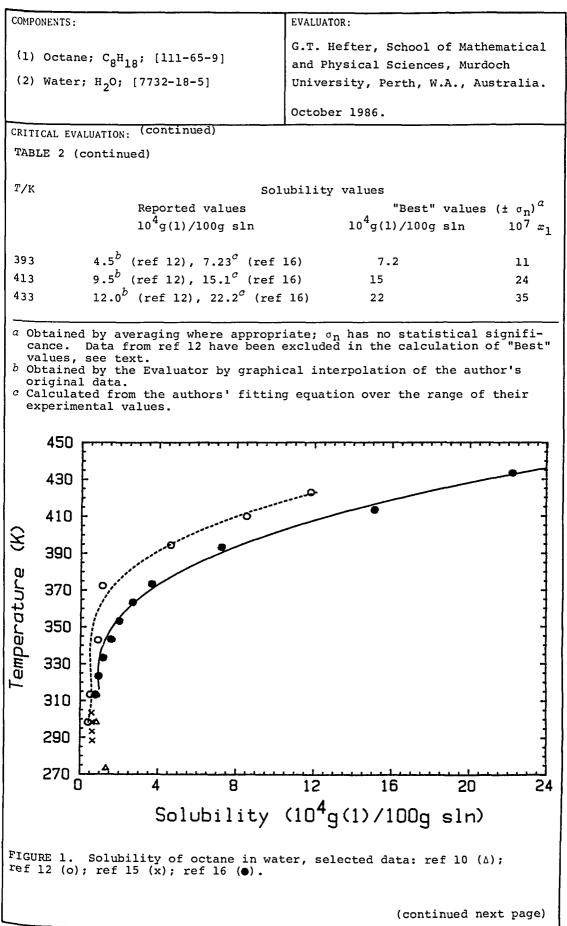
eratures the values of Price (ref 12) are also considerably lower than those of Heidman *et al.* (ref 16). In the absence of confirmatory studies, it is not reasonable to reject Price's data outright but they have not been used in the calculation of "Best" values. Application of the van't Hoff equation to both data sets gives values of  $\Delta H_{sln} = -3.3$  (ref 12) and +13.3 (ref 16) kJ mol⁻¹ and  $\Delta C_{p,sln} = 568$  (ref 12) and 284 (ref 16) J K⁻¹ mol⁻¹. Neither set of values are close to those reported for related systems although those of Heidman *et al.* are somewhat more reasonable.

At other temperatures the data of Fühner (ref 1), Nelson and De Ligny (ref 6), and Budantseva *et al*. (ref 11) are markedly higher than all other studies and are therefore rejected. All the remaining data are summarized in Table 2 and selected data are plotted in Figure 1.

It is interesting to note that the averaged "Best" value at 298K is very close to the value which would be predicted by an extrapolation of the lower n-alkane solubilities.

T/K	Solubility values		
	Reported values	"Best" values	$(\pm \sigma_n)^a$
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln	10 ⁷ <i>x</i> 1
273	1.35 (ref 10)	1.4	2.2
293	0.628 (ref 15)	0.63	0.99
298	0.66 (ref 5), 0.70 (ref 9), 0.85 (ref 10), 0.615 (ref 15)	0.71 ± 0.09	1.1
303	0.46 ^b (ref 12), 0.612 (ref 15)	0.61	0.96
313	$0.52^{b}$ (ref 12), $0.80^{c}$ (ref 16)	0.8	1.3
323	0.61 ^{$b$} (ref 12), 0.96 ^{$c$} (ref 16)	1.0	1.6
333	$0.74^{b}$ (ref 12), $1.2^{c}$ (ref 16)	1.2	1.9
343	$0.91^{b}$ (ref 12), $1.5^{c}$ (ref 16)	1.5	2.4
353	$1.0^{b}$ (ref 12), 1.99 c (ref 16)	2.0	3.2
363	$1.1^{b}$ (ref 12), 2.67 ^c (ref 16)	2.7	4.3
373	$1.2^{b}$ (ref 12), 3.66 c (ref 16)	3.7	5.8

## TABLE 2: Tentative Values of the Solubility ofOctane (1) in Water (2)



COMPONENTS:EVALUATOR:(1) Octane; C8H18; [111-65-9]G.T. Hefter, School of Mathematical<br/>and Physical Sciences, Murdoch<br/>University, Perth, W.A., Australia.(2) Water; H2O; [7732-18-5]University, Perth, W.A., Australia.

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN OCTANE (1)

Only limited data are available for the solubility of water in *n*-octane and agreement amongst independent determinations is only fair. The datum of Black *et al.* (ref 2) is much higher than all other values and is therefore rejected. The remaining data are collected in Table 3 and plotted in Figure 2.

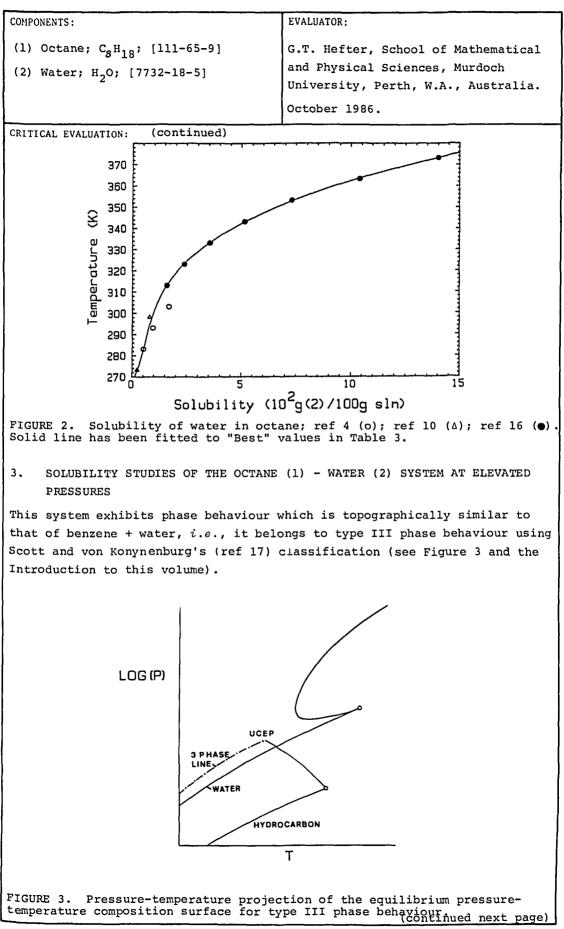
TABLE 3: Tentative Values of the Solubility ofWater (2) in Octane (1)

T/K	Solubili	ty values.	
	Reported values	"Best" values (:	± σ _n ) ^α
	10 ² g(2)/100g sln	10 ² g(2)/100g sln	$10^4 x_2$
273	0.23 (ref 9)	0.2	1
283	0.51 (ref 4)	0.5	3
293	0.95 (ref 4), 0.68 (ref 10)	0.8 ± 0.1	5
298	l.26 ^b (ref 4), 0.79 (ref 9)	1.0 ± 0.2	6
303	1.68 (ref 4)	1.7	11
313	1.58° (ref 14)	1.6	10
323	2.40 [°] (ref 14)	2.4	15
333	3.54 [°] (ref 14)	3.5	22
343	5.14 [°] (ref 14)	5.1	32
353	7.30 [°] (ref 14)	7.3	46
363	$10.2^{c}$ (ref 14)	10	63
373	14.0 [°] (ref 14)	14	89

a Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance.

 b Obtained by graphical interpolation (Evaluator) of authors' original data.
 c Calculated (Evaluator) from fitting equation given by authors, over the range of their experimental values.

(continued next page)



COMPONENTS:	EVALUATOR:
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	October 1986.

CRITICAL EVALUATION: (continued)

Quantitative solubility data on the octane - water system at elevated pressures have been reported in the studies listed in Table 4.

# TABLE 4. Solubility Studies of the Octane (1) - Water (2) System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Roof (ref 8)	_a	_a	_a
Price (ref 12)	_ <i>b</i>	298-423	(l) in (2)
Skripka (ref 14)	3.5-78.5	498-538	(2) in (1)
Heidman et al. (ref 16)	$0.01 - 8.9^{b}$	311-539	mutual

a Critical point of unspecified composition. b Along the three-phase line.

As can be seen from Table 4 data have not generally been obtained under comparable conditions, making Critical Evaluation difficult. However, it may be noted that the solubility of 9.95 g(2)/100g sln of water in octane at 7.4 MPa and 538.2 K reported by Skripka (ref 14) differs markedly from the value of 14.9 g(2)/100g sln reported at 7.41 MPa and 539.1 K by Heidman *et al.* (ref 16). Further studies are necessary before any preference can be expressed for either data set. Previous mention (Section 1 above) has already been made of the fact that the solubilities of octane in water reported by Heidman *et al.* (ref 16) are much higher than those of Price (ref 12).

On the other hand the properties of the critical end point (Figure 3) reported by Roof: 7.41 MPa and 540.4 K, are in good agreement with those reported by Heidman *et al.* (ref 16): 7.41 MPa and 539.1 K.

COMPONENTS :	EVALUATOR:		
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	G.T. Hefter, School of Mathematical		
(2) Water; $H_2O$ ; [7732-18-5]	and Physical Sciences, Murdoch		
$(2)$ water, $n_20$ , $[7732-10-5]$	University, Perth, W.A., Australia.		
	October 1986.		
CRITICAL EVALUATION: (continued)			
REFERENCES			
1. Fühner, H. Chem. Ber. <u>1924</u> , 52	² , 510-5.		
2. Black, C.; Joris, G.G.; Taylor,	H.S. J. Chem. Phys. <u>1948</u> , 16, 537-48.		
3. Baker, E.G. Geochim. Cosmochim.	Acta <u>1960</u> , <i>19</i> , 309-17.		
<ol> <li>Englin, B.A., Plate, A.F.; Tugol Tekhnol. Topl. Masel <u>1965</u>, 10,</li> </ol>	ukov, V.M.; Pyranishnikova, M.A. 42-6.		
5. McAuliffe, C. J. Phys. Chem.	<u>966</u> , 70, 1267-75.		
<ol> <li>Nelson, H.D.; De Ligny, C.L. Re 528-44.</li> </ol>	c. Trav. Chim. Pays-Bas <u>1968</u> , 87,		
7.* Alwani, Z.; Schneider, G.M. Ber 294-301.	. Bunsenges. Phys. Chem. <u>1969</u> , 73,		
8. Roof, J.G. J. Chem. Eng. Data	<u>1970</u> , <i>15</i> , 301-3.		
<ol> <li>Krasnoshchekova, P.Y.; Gubergrit 885-7.</li> </ol>	s, M.Y. Neftekhimiya <u>1973</u> , 13,		
10. Polak, J.; Lu, B.C-Y. Can. J. C	hem. <u>1973</u> , 51, 4018-23.		
11. Budantseva, L.S.; Lesteva, T.M.; 50, 1344, Deposited doc. 1976,	Nemstov, M.S. <i>2h. Fiz. Khim</i> . <u>1976</u> , VINITI 437-76.		
12. Price, L.C. Am. Assoc. Petrol.	Geol. Bull. <u>1976</u> , 60, 213-44.		
13. Krzyzanowska, T.; Szeliga, J. M	afta (Katowice) <u>1978</u> , 34, 413-7.		
14. Skripka, V.G. Tr. Vses. Neftega 139-51.	. Skripka, V.G. Tr. Vses. Neftegasov. Nauch-Issled. Inst. <u>1976</u> , 61,		
15. Jonsson, J.A.; Vejrosta, J.; Nov 279-86.	ak, J. Fluid Phase Equil. <u>1982</u> , 9,		
<pre>16. Heidman, J.L.; Tsonopoulos, C.; <u>1985</u>, 31, 376-84.</pre>	Brady, C.J.; Wilson, G.M. A.I.Ch.E.J.		
17. Scott, R.L.; van Konynenburg, P. <u>1980</u> , A298, 495.	H. Phil. Trans. Roy. Soc. London		
ACKNOWLEDGEMENT			
The Evaluator thanks Dr Brian Clare for the graphics.			
*NOTE ADDED IN PROOF			
Delete ref 7.			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Fühner, H.
(2) Water; H ₂ O; [7732-18-5]	Ber. Dtsh. Chem. Ges. <u>1924</u> , 57, 510-5.
VARIABLES:	PREPARED BY:
One temperature: 16°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of octane in water at 0.002 mL(1)/100 mL sln or 0.0014 g(1) The corresponding mole fraction, $x_1$ , is 0.22 x $10^{-5}$ .	/100 g sln.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a stoppered measuring cylinder pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100 or 1000 cm ³ of (2) until a completely clear solution was obtained at the experimental tem- perature.	<ul> <li>(1) source not specified; commer- cial grade; used as received.</li> <li>(2) not specified.</li> </ul>
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Black, C.; Joris, G.G.; Taylor, H.S.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Phys. <u>1948</u> , 16, 537-43.
VARIABLES:	PREPARED BY:
One temperature: 20°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of water in octane at saturation pressure of 1 atm was report The corresponding mass percent and mo by the compiler are 0.0142 g(2)/100 g	prted to be 0.0142 g(2)/100 g(1). Dle fraction, $x_2$ , calculated
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The method described in ref l in which tritium oxide acts as a tracer, Was used. Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred in the counter through equilibration with ethanol vapor.	(1) Ohio State University under an
	ESTIMATED ERROR:
	soly. a few percent (type of error not specified).
	REFERENCES:
	l. Joris, G.G.; Taylor, H.S. J. Chem. Phys. <u>1948</u> , 16, 45.

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Baker, E.G.		
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1960</u> , 19, 309-17.		
VARIABLES:	PREPARED BY:		
One temperature: not specified.	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
The solubility of octane in water was 0.09 x 10 ⁻⁶ mL(1)/mL(2).	a reported to be		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The solubility of (1) in (2) was determined after ultrafiltration using the procedure described in ref 1.	not specified.		
	ESTIMATED ERROR:		
	not specified.		
	REFERENCES:		
	<ol> <li>Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprint 1958, 3, N°4, C61.</li> </ol>		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Englin, B.A.; Plate, A.F.; Tugolu		
(2) Water; H ₂ O; [7732-18-5]	V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.		.A.
2			l <u>1965</u> ,
VARIABLES:	PREPARED BY:		
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirs		lait-Pirso
EXPERIMENTAL VALUES:			
Solubility of wa			
t/°C g(2)/1	00 g sln 10	0 ⁴ x ₂	(compiler)
10 0.	0051	3.24	
		6.03	
30 0.	0168 10	0.65	
	INFORMATION		
	INFORMATION SOURCE AND PURITY OF MATER	IALS:	
ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into		IALS:	
ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal-	SOURCE AND PURITY OF MATER	IALS :	
ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated	SOURCE AND PURITY OF MATER	IALS :	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURITY OF MATER	IALS :	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURITY OF MATER	IALS:	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURITY OF MATER (1) not specified. (2) not specified.	IALS:	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURITY OF MATER (1) not specified. (2) not specified. ESTIMATED ERROR:	IALS :	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURITY OF MATER (1) not specified. (2) not specified. ESTIMATED ERROR: not specified.	IALS:	
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2)	SOURCE AND PURITY OF MATER (1) not specified. (2) not specified. ESTIMATED ERROR: not specified.	IALS:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of octane in water at	25°C was reported to
be 0.66 mg (1)/kg sln.	
The corresponding mole fraction, $x_1$ ,	calculated by the compiler,
is $1.04 \times 10^{-7}$ .	
The same value is also reported in re	ers 1 and 2.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250 mL glass bottle, 10-20 mL	(1) Phillips Petroleum Co.; 99+% purity; used as received.
of (1) was vigorously shaken for 1 hr or magnetically stirred for	purity; used as received.
1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution	(2) distilled.
was allowed to stand for 2 days to	
permit separation of small (1) drop- lets. Absence of emulsion was	
checked microscopically. A 50 µL	
sample of the (1) saturated water was withdrawn with a Hamilton	
Syringe and injected into the frac- tionator of the gas chromatograph.	ESTIMATED ERROR:
A hydrogen-flame ionization detector	
was used. Many details are given in the paper.	deviation from mean)
	REFERENCES:
	1. McAuliffe, C. Nature (London)
	<u>1963</u> , 200, 1092.
	2. McAuliffe, C. Am. Chem. Soc.,
	Div. Petrol. Chem. <u>1964</u> , 9, 275.

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Nelson, H.D.; De Ligny, C.L.
(2) Water, H ₂ O; [7732-18-5]	Rec. Trav. Chim. Pays-Bas <u>1968</u> , 87, 528-44.
VARIABLES:	PREPARED BY:
Temperature: 5-45°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	L
Solubility of oc	tane in water
$t/^{\circ}C$ $10^{7}x$	l mg(l)/kg sln (compiler)
5.0 2.6 ±	0.6 1.65
15.0 1.4 ±	
45.0 2.9 ± 0	0.6 1.84
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The saturation vessel is drawn in	(1) Fluka purum.
the original paper. (2) was satu-	· · · ·
rated with (1) via the vapor phase: a few drops of (1) were put on the	(2) tap-water was refluxed for 8 hours in the presence of KMnO ₄
bottom of a tight-fitting flask containing a small flask filled with	and KOH and distilled. The "whole process was repeated once
water. Complete saturation was reached by shaking overnight in an	more.
upright position. Samples were	
taken from the aqueous solution with a microsyringe through the	
septum and injected into the gas chromatograph equipped with a flame	ESTIMATED ERROR:
ionization detector. The gas chro- matographic conditions are described in the paper.	soly.: error given above (standard deviation)
	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:			
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya 1973, 13, 885-7.			
VARIABLES:	PREPARED BY:			
One temperature: 25°C	A. Maczynski			
EXPERIMENTAL VALUES: The solubility of octane in water at $x_1 = 1.0 \times 10^{-7}$ . The corresponding mass percent calcul 7.0 x $10^{-5}$ g(1)/100 g sln.				
AUXILIARY	INFORMATION			
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:			
A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigor- ously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air,	<ul> <li>(1) source not specified; CP reagent; purity not specified.</li> <li>(2) distilled.</li> </ul>			
and the (1)-saturated air was	ESTIMATED ERROR:			
analyzed by glc.	not specified.			

	14:		
COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Polak, J.; Lu, B.C-Y.		
(2) Water; H ₂ O; [7732-18-5]	Can. J. Chem. <u>1973</u> , 51, 4018-23.		
VARIABLES:	PREPARED BY:		
Temperature: 0-25°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
SA EXITENTAL VALUES.			
Solubility of oc	stane in water		
t/°C mg(l)/kg	$x_1$ (compiler)		
0 ^a 1.35	_		
25 ^b 0.85	$1.34 \times 10^{-7}$		
Solubility of wa	ter in octane		
t/°C mg(2)/kg	sln $x_2$ (compiler)		
	$1.46 \times 10^{-4}$		
25 ^b 79 ^e	5.01 $\times$ 10 ⁻⁴		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titra- tion. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetical- ly for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.	<pre>(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled. ESTIMATED ERROR: temp. a) ± 0.02°C; b) ± 0.01°C soly. c) ± 4%; d) ± 4.7%; e) ± 3.1% (mean) REFERENCES:</pre>		

COMPONENTS:	ODICINAL NEACHDENENTS.		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S.		
2	Zh. Fiz. Khim. <u>1976</u> , 50, 1344. Deposited doc. <u>1976</u> , VINITI 437-76.		
VARIABLES:	PREPARED BY:		
One temperature: 20°C	A. Maczynski		
EXPERIMENTAL VALUES:			
The solubility of octane in water at $x_1 \approx 2 \times 10^{-7}$ .	20°C was reported to be		
The corresponding mass percent calcu about 0.0001 g(1)/l00 g sln.	lated by the compiler is		
The solubility of water in octane at $x_2 = 4.3 \times 10^{-4}$ .	20°C was reported to be		
The corresponding mass percent calcu 0.007 g(2)/100 g sln.	lated by the compiler is		
	INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
Nothing specified in the paper.	(1) not specified.		
	(2) not specified.		
	1		
	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES :		

L.

APONENTS :		ORIGINAL MEASUREMENTS:	
) Octane; C ₈ H ₁₈ ; [111-65-9]		Price, L.C.	
2) Water; H ₂ O; [7732-18-5]		Ат. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.	
RIABLES:	······································		
		PREPARED BY:	
emperature: 2	5-149.5°C	F. Kapuku	
PERIMENTAL VALUE	S:	<u> </u>	
Sol	ubility of octane in wa	ter at system pressu	ce
t/°C	mg(l)/kg(2)	g(l)/l00 g sln (compiler)	10 ⁷ x1 (compiler)
25.0	0.431 ± 0.012	0.0000431	0.680
40.1	$0.524 \pm 0.021$	0.0000524	0.826
69.7	0.907 ± 0.042	0.0000907	1.43
99.1	1.12 ± 0.07	0.000112	1.77
121.3	4.62 ± 0.22	0.000462	7.29
136.6	8.52 ± 0.34	0.000852	13.4
149.5	11.80 ± 0.7	0.00118	18.6
		INFORMATION	
ETHOD /AP PARATUS / P	ROCEDURE :	SOURCE AND PURITY OF MAT	•
Noom-temperatu letermined by	ROCEDURE: re solubilities were use of screw-cap test		•
Room-temperatu letermined by tubes. The (1	ROCEDURE: re solubilities were use of screw-cap test ) phase floated on top	SOURCE AND PURITY OF MAT	•
Room-temperatu letermined by cubes. The (1 of (2) and ins co 4 days) of ligh-temperatu carried out in chromatograph. contained in 7 stainless stee Modified Micro	PROCEDURE: re solubilities were use of screw-cap test ) phase floated on top ured saturation (in 2 the aqueous phase. re solubility work was the ovens of the gas The solutions were 5 mL double ended 1 sample cylinders. Linear Valves sealed	SOURCE AND PURITY OF MAT (1) Phillips Petrole 99+%.	•
Room-temperatu letermined by cubes. The (1 of (2) and ins to 4 days) of ligh-temperatu arried out in chromatograph. contained in 7 stainless stee fodified Micro the bottom of	PROCEDURE: re solubilities were use of screw-cap test ) phase floated on top ured saturation (in 2 the aqueous phase. re solubility work was the ovens of the gas The solutions were 5 mL double ended 1 sample cylinders.	SOURCE AND PURITY OF MAT (1) Phillips Petrole 99+%.	•
Coom-temperatu letermined by cubes. The (1 of (2) and ins co 4 days) of ligh-temperatu carried out in chromatograph. contained in 7 stainless stee Modified Micro che bottom of Lowed syringe during samplin transferred to equipped with	PROCEDURE: re solubilities were use of screw-cap test ) phase floated on top ured saturation (in 2 the aqueous phase. re solubility work was the ovens of the gas The solutions were 5 mL double ended 1 sample cylinders. Linear Valves sealed the cylinder and al-	SOURCE AND PURITY OF MAT (1) Phillips Petrole 99+%. (2) distilled.	eum Company;
Coom-temperatu letermined by cubes. The (1 of (2) and ins co 4 days) of ligh-temperatu carried out in chromatograph. contained in 7 stainless stee Modified Micro che bottom of Lowed syringe during samplin transferred to equipped with	PROCEDURE: re solubilities were use of screw-cap test ) phase floated on top ured saturation (in 2 the aqueous phase. re solubility work was the ovens of the gas The solutions were 5 mL double ended 1 sample cylinders. Linear Valves sealed the cylinder and al- access to the solution g. The sample is then the gas chromatograph dual flame ionization	SOURCE AND PURITY OF MAT (1) Phillips Petrolo 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1°C	eum Company;
Coom-temperatu letermined by cubes. The (1 of (2) and ins co 4 days) of ligh-temperatu carried out in chromatograph. contained in 7 stainless stee Modified Micro che bottom of cowed syringe during samplin transferred to equipped with letectors. Ma	PROCEDURE: re solubilities were use of screw-cap test ) phase floated on top ured saturation (in 2 the aqueous phase. re solubility work was the ovens of the gas The solutions were 5 mL double ended 1 sample cylinders. Linear Valves sealed the cylinder and al- access to the solution g. The sample is then the gas chromatograph dual flame ionization	<pre>SOURCE AND PURITY OF MAT (1) Phillips Petrole 99+%. (2) distilled.  ESTIMATED ERROR: temp. ± 1°C soly. range of value</pre>	eum Company;
Coom-temperatu letermined by cubes. The (1 of (2) and ins co 4 days) of ligh-temperatu carried out in chromatograph. contained in 7 stainless stee Modified Micro che bottom of cowed syringe during samplin transferred to equipped with letectors. Ma	PROCEDURE: re solubilities were use of screw-cap test ) phase floated on top ured saturation (in 2 the aqueous phase. re solubility work was the ovens of the gas The solutions were 5 mL double ended 1 sample cylinders. Linear Valves sealed the cylinder and al- access to the solution g. The sample is then the gas chromatograph dual flame ionization	<pre>SOURCE AND PURITY OF MAT (1) Phillips Petrole 99+%. (2) distilled.  ESTIMATED ERROR: temp. ± 1°C soly. range of value</pre>	eum Company;
Coom-temperatu letermined by cubes. The (1 of (2) and ins co 4 days) of ligh-temperatu carried out in chromatograph. contained in 7 stainless stee Modified Micro che bottom of cowed syringe during samplin transferred to equipped with letectors. Ma	PROCEDURE: re solubilities were use of screw-cap test ) phase floated on top ured saturation (in 2 the aqueous phase. re solubility work was the ovens of the gas The solutions were 5 mL double ended 1 sample cylinders. Linear Valves sealed the cylinder and al- access to the solution g. The sample is then the gas chromatograph dual flame ionization	<pre>SOURCE AND PURITY OF MAT (1) Phillips Petrole 99+%. (2) distilled.  ESTIMATED ERROR: temp. ± 1°C soly. range of value</pre>	eum Company;

COMPONENTS: ORIGINAL MEASUREMENTS: Skripka, V.G. Tr. Vses. Neftegazov. Nauch. Issled. Inst. <u>1976</u>, 61, 139-51. (1) Octane; C₈H₁₈; [111-65-9] (2) Water, H₂O; [7732-18-5] Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. 1973, 47, 1035. VARIABLES: PREPARED BY: Temperature: 225-265°C A. Maczynski Pressure: 3.5-78.5 MPa EXPERIMENTAL VALUES: Solubility of water in octane  $p/kg cm^{-2}$ t/°C g(2)/100 g sln p/MPa *x*2 (compiler) (compiler) 225 36 3.5 0.166 3.04 100 9.8 0.137 2.44 200 19.6 1.89 0.109 300 29.4 0.098 1.68 39.2 0.091 400 1.55 500 49.0 0.088 1.50 1.42 58.8 0.084 600 0.080 1.35 700 68.6 78.5 0.075 1.26 800 0.216 240 50 4.9 4.16 3.63 100 9.8 0.193 200 19.6 0.164 3.00 29.4 0.149 300 2.69 400 39.2 0.140 2.50 500 49.0 0.132 2.34 600 58.8 0.126 2.22 700 68.6 0.122 2.14 800 78.5 0.117 2.05 (continued) AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The experimental technique was described in ref 1. No details (1) source not specified, chemical reagent grade; purity not specified; used as received. reported in the paper. (2) distilled. ESTIMATED ERROR: not specified. **REFERENCES:** 1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. Gazov. Prom. <u>1971</u>, 4, 6.

	1) Octane; C ₈ H ₁₈ ; [111-65-9] 2) Water; H ₂ O; [7732-18-5]		Skripka, V.G. Tr. Vses. Neftegazov. Nauch. Issled. Inst. <u>1976</u> , 61, 139-51.		
		Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. <u>1973</u> , 47, 1035.			
t/°C	$p/kg \text{ cm}^{-2}$	p/MPa (compiler)	<i>x</i> ²	g(2)/100 g sln (compiler)	
265	75 100 200 300 400 500 600 700 800	7.4 9.8 19.6 29.4 39.2 49.0 58.8 68.6 78.5	0.412 0.350 0.254 0.224 0.207 0.194 0.183 0.172 0.163	9.95 7.83 5.10 4.35 3.95 3.66 3.41 3.19 2.98	

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Krzyzanowska, T.; Szeliga, J.		
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.		
-			
VARIABLES:	PREPARED BY:		
0			
One temperature: 25°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
The solubility of octane in water at 25°C was reported			
to be 0.431 mg(1)/kg(2).	to be $0.431 mg(1)/kg(2)$ .		
The corresponding mass percent and ma	ole fraction, $x_{\cdot}$ , calculated		
The corresponding mass percent and mole fraction, $x_1$ , calculated by compiler are 4.31 x 10 ⁻⁵ g(1)/100 g sln and 6.80 x 10 ⁻⁸ .			
by complier are 4.31 x 10 $^{-}$ g(1)/100 g sln and 6.80 x 10 $^{\circ}$ .			

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system.

AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>
	ESTIMATED ERROR: soly. 0.02 mg(1)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES :

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Octane; C ₈ H ₁₈ ; [111-65-9]		Jonsson, J.A.; Vejrosta, J.; Novak, J.		
(2) Water; H.	20; [7732-18-5]		1000 0 070 00	
		Fluid Phase Equil.	<u>1982</u> , 9, 279-86.	
VARIABLES:		PREPARED BY:		
Temperature:	15-35°C	G.T. Hefter		
EXPERIMENTAL VAL	UES:	<u> </u>		
	Solubility of	octane in water		
t/°C	mg(1)/kg sln	10 ⁵ g(1)/100g sln	$10^{7}x_{1}$	
<i>t</i> /-C		(compiler)	(compiler)	
15	0.653	6.53	1.03	
20	0.628	6.28	0.99	
25 30	0.615 0.612	6.15 6.12	0.97 0.96	
30	0.620	6.20	0.98	
		····		
	AUXILIARY	INFORMATION		
METHOD/APPARATUS	/PROCEDURE:	SOURCE AND PURITY OF M	ATERIALS:	
were measured portion of wa	rtition coefficients 1 by saturating a 1ter by a stream of 2aining a known vapour	<pre>(1) Fluka, &gt; 99.8% received. (2) Not specified.</pre>		
concentration equilibration was adsorbed trap and the by gas chroma	n of (1). After n, the dissolved (1) in a porous polymer entrapped (1) analysed atography. The method s are described in			
[		ESTIMATED ERROR:		
		Not specified.		
		REFERENCES:		
		1. Vejrosta, J.;	Fluid Phase Equil.	

COMPONENTS: ORIGINAL MEASUREMENTS: Heidman, J.L.; Tsonopoulos, C.; (1) Octane; C₈H₁₈; [111-65-9] (2) Water, H₂O; [7732-18-5] Brady, C.J.; Wilson, G.M. A. I. Ch. E. J. 1985, 31, 376-84. VARIABLES: PREPARED BY: Temperature: 311-553 K G.T. Hefter Pressure: 0.01-7.4 MPa EXPERIMENTAL VALUES: Solubility of octane in water 10² g(1)/100 g sln  $10^5 x_1$ T/K p /MPa (compiler) 0.0103^a 310.9 0.012 0.0076 0.117^a 0.048 0.030 366.5 0.24 422.0 0.655 0.38 4.0 2.5 479.5 2.51 35 22 536.1 7.03 60^b 552.8 8.86 38 a Estimated by the authors from pure component data b Above three-phase equilibrium point. (continued) AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: (1) Aldrich 99+ mol %; water free Experimental procedure was similar to purity ≥ 99.9 mol %, checked that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. by gas chromatography. Critical points were determined by the (2) Distilled; no details given. synthetic method using visual observ-ation. This aspect of the procedure is discussed in detail in the paper. ESTIMATED ERROR: soly. ± 5%, relative precision of replicate analyses. temp. not stated. press. ± 1%; type of error not stated. **REFERENCES:** Tsonopoulos, C.; Wilson, G.M. A. I. Ch. E. J. <u>1983</u>, 29, 990-9.

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(1) Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]
(2) Water, H<sub>2</sub>O; [7732-18-5]
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(continued)

#### Solubility of water in octane

<i>T</i> /K	p /MPa	$10^2 x_2$	g(2)/100 g sln (compiler)
310.9	0.0103 ^{<i>a</i>}	0.100	0.0158
366.5	0.117	0.62	0.098
422.0	0.655	3.94	0.622
477.6	- ^b	12.6	2.22
533.1	<b>-</b> ^b	38.7	9.05
539.1 ⁰	7.41	52.7 [°]	14.9
$550.4^{d}$	-	54.9 ^d	16.1

a Estimated by the authors from pure component data.

b Not specified.

c Three phase critical point.

d Above three phase critical point.

The three phase critical point was reported to be 539.1  $\pm$  0.6 K, 7.37  $\pm$  0.04 MPa and  $x_1 = 4.61 \times 10^{-4}$  (0.292 g(1)/100 g sln, compiler).

The authors also report equations which fit their own and literature data over the range 273-539 K, viz.

 $\ln x_1 = -343.1497 + 13862.49/T + 49.24609 \ln T$   $\ln x_2 = -0.66037 - 7.1130 (T_p^{-1} - 1) - 0.67885 (1 - T_p^{-1})^{1/3}$  $- 1.43381 (1 - T_p^{-1})$ 

where  $T_p = T/539.1$ 

COMPONENTS:		EVALUATO	DR:	
<pre>(1) Octane; C₈H₁₈; [111-65- (2) Seawater</pre>	9]	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA		
		Decem	per 1982	
CRITICAL EVALUATION:				· · · · · · · · · · · · · · · · · · ·
The solubility of octane (1 works:	) in seawa	ter (2)	has been report	ted in two
Authors	Method	T/K	Salinity. g salts/kg sln	g(l)/100 g sl
Krasnoshchekova and Gubergrits (ref 1)	GLC	298	6	$2.5 \times 10^{-4}$
Freegarde <i>et al</i> . (ref 2)	GLC	?	?	$1 \times 10^{-4}$
Because temperature and sal et al. are rejected. The w	value of Kr	asnoshc	hekova and Gube	rgrits is con-
sidered doubtful since it i solubility of octane in pur	e water at	298 K. ANE (1)	IN SEAWATER (2)	
sidered doubtful since it i solubility of octane in pur <u>SOLUBII</u>	e water at	298 K. ANE (1) TFUL VA	IN SEAWATER (2) LUE	<u>L</u>
sidered doubtful since it i solubility of octane in pur	e water at	298 K. ANE (1)	IN SEAWATER (2) LUE sln g(2	

- Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u>, 13, 885-8.
- 2. Freegarde, M.; Hatchard, C.G.; Parker, C.A. Lab. Pract. <u>1971</u>, 20, 35-40.

CONDONENTE	ORIGINAL MEASUREMENTS:
COMPONENTS:	
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Freegarde, M.; Hatchard, C.G.; Parker, C.A.
(2) Seawater (composition not specified)	Lab Pract. <u>1971</u> , 20, 35-40.
VARIABLES:	PREPARED BY:
Temperature, pressure, salinity not given.	M. Kleinschmidt and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of octane was reported	to be 1.0 mg/L. The
corresponding mass percent and mole fi	+
by the compilers are 1.0 x $10^{-4}$ g(1)/2	100 g sln and 1.6 x $10^{-7}$ ,
assuming a solution density of 1.02 kg	g/L.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
None given except that analysis was done using gas chromatography.	not given.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:
	REFERENCES;

COMPONENTS:

ORIGINAL MEASUREMENTS: Krasnoshchekova, R.Ya.; (1) Octane; C₈H₁₈; [111-65-9] Gubergrits, M.Ya. (2) Seawater Neftekhimiya 1<u>973</u>, 13, 885-8. VARIABLES: PREPARED BY: One temperature: 25°C M. Kleinschmidt Salinity: 6 g/kg sln **EXPERIMENTAL VALUES:** The solubility of octane in seawater was reported to be 2.5 x  $10^{-4}$  g(1)/100 g sln. and the corresponding mole fraction,  $x_{1} = 4.0 \times 10^{-7}$ . AUXILIARY INFORMATION METHOD / APPARATUS / PROCEDURE : SOURCE AND PURITY OF MATERIALS: (1) "chemically pure" A saturated solution was prepared by vigorously stirring hydrocarbon (2) distilled water plus salt (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature mixture. controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding ESTIMATED ERROR: solution concentration calculated. not specified. **REFERENCES:** 

COMPONENTS :	EVALUATOR:
(1) Indan; C ₉ H ₁₀ ; [496-11-7] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences Warszawa, Poland.
	February 1986.

Quantitative solubility studies for indam (1) in water (2) have been reported in the publications listed in Table 1.

	TABLE 1.	Quantitative Solubility Indan (1) in Water (2)	Studies of
	Reference	T/K	Method
Price (ref	1)	298	GLC
Mackay and	Shiu (ref 2)	298	spectrofluorometric

The original data in these publications are compiled in the Data Sheets immediately following this evaluation. No data have been reported on the solubility of water in indan.

The data of Price (ref 1) and Mackay and Shiu (ref 2) are in good agreement (Table 2) although the relative uncertainty (± 10%) is too large for the mean to be Recommended given the relatively high solubility. Further studies are required.

TABLE 2:	Tentative Value of the Solubility of
	Indan (1) in Water (2)

<i>Т/</i> К	Solubility	y value	
	Reported value 10 ² g(1)/100g sln	"Best" value (±ơ _n ) 10 ² g(1)/100g sln	10 ⁵ x ₁
298	0.889 (ref l), l.091 (ref 2)	1.0 ± 0.1	1.5

REFERENCES

1. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.

2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

COMPONENTS:ORIGINAL MEASUREMENTS:(1) Indan; C9H10; [496-11-7]Price, L.C.(2) Water; H20; [7732-18-5]Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.VARIABLES:PREPARED BY:One temperature: 25°CM.C. Haulait-Pirson

#### EXPERIMENTAL VALUES:

The solubility of indam in water at 25°C and at system pressure was reported to be 88.9 mg(1)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 0.00889 g(1)/ 100 g sln and 1.35 x 10⁻⁵.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de- tails are given in the paper.	<pre>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 2.7 mg(1)/kg(2) REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
	Mackay, D.; Shiu, W.Y.
(1) Indan; $C_{9H_{10}}$ ; [496-11-7]	
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of indan in water at to be 109.1 mg(1) dm ⁻³ sln and $x_1 =$	$1.665 \times 10^{-5}$ .
The corresponding mass percent calcu is 0.01091 g(1)/100 g sln.	lated by the compiler
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.</li> <li>(2) doubly distilled.</li> </ul>
analysis. Many details are given	ESTIMATED ERROR:
in the paper.	soly. $\pm$ 1.02 mg(1) dm ⁻³ sln (maximum deviation from several determina-tions).
	REFERENCES :

COMPONENTS :	EVALUATOR:
(1) 1,2,3-Trimethylbenzene; C ₉ H ₁₂ ; [526-73-8]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch
(2) Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia.
	December 1986

Quantitative solubility data for 1,2,3-trimethylbenzene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1,2,3-trimethylbenzene.

# TABLE 1: Quantitative Solubility Studies of1,2,3-Trimethylbenzene (1) in Water (2)

Reference	T/K	Method
Sutton and Calder (ref 1)	298	GLC
Sanemasa <i>et al</i> . (ref 2)	288-318	spectrophotometry

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The available data are summarized in Table 2. At 298K, the only temperature where comparison is possible, the data of Sutton and Calder (ref 1) and Sanemasa  $et \ al$ . (ref 2) are in reasonable agreement (Table 2) and their average may be considered as the Tentative solubility.

At other temperatures, only the data of Sanemasa  $et \ al$ . are available so no Critical Evaluation is possible. Nevertheless, it may be noted that for other hydrocarbons in water the data of Sanemasa  $et \ al$ . are normally reliable.

TABLE 2: Tentative Values of the Solubility of 1,2,3-Trimethylbenzene (1) in Water (2)

T/K	Solubili Reported values 10 ³ g(1)/100g sln	ity values "Best" values ( 10 ³ g(1)/100g sln	$(\pm \sigma_n)^a$
288	5.99 (ref 2)	6.0	9.0
298	7.52 (ref 1), 6.27 (ref 2)	6.9 ± 0.5	10
308	7.22 (ref 2)	7.2	11
318	8.52 (ref 2)	8.5	13
1			

a Obtained by averaging where appropriate;  $\sigma_{\rm n}$  has no statistical significance.

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(continued next page)

COMPONENTS:	EVALUATOR:
(1) 1,2,3-Trimethylbenzene; C ₉ H ₁₂ ; [526-73-8] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. December 1986.

REFERENCES

- 1. Sutton, C.; Calder, J.A. J. Chem. Eng. Data <u>1975</u>, 20, 320-2.
- 2. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62.

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1,2,3-Trimethylbenzene; C₉H₁₂; [526-73-8] (2) Water; H₂O; [7732-18-5]</pre>	Sutton, C.; Calder J.A. J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of 1,2,3-trimethylben: to be 75.2 mg(1)/kg(2). The correspondence $x_1$ , calculated by the compilers are of 1.126 x 10 ⁻⁵ .	onding mass percent and mole fraction,
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chromatography.	<ol> <li>Aldrich Chemical Co. or Matheson Coleman and Bell purified by distillation through a Vigreaux Column; 94.4% purity determined by gas chromatography.</li> <li>Distilled.</li> </ol>
	ESTIMATED ERROR:
	Temp. ±0.1°C
	Soly. 0.6 (the standard deviation of the mean for six replicates).
	REFERENCES :

COMPONENTS :	····	ORIGINAL MEASUREMENTS:	
JOHF UNEN 15 .			м
(1) 1,2,3-Trin	methylbenzene; C ₉ H ₁₂ ;	Sanemasa, I.; Araki,	
[526-73-8	]	Deguchi, T.; Nagai, H Bull. Chem. Soc. Jpn. <u>19</u>	
(2) Water; H ₂ (	D; [7732-18-5]	butt. onem. 500. spn. <u>13</u>	<u>, , , , , , , , , , , , , , , , , , , </u>
VARIABLES:		PREPARED BY:	
Temperature:	15-45°C	G.T. Hefter	
EXPERIMENTAL VALU	JES:	I	
r	the solubility of 1,2,3-t	rimethylbenzene in wat	er
<i>t /</i> °C	10 ⁴ mol(1)/dm ³ sln	10 ³ g(1)/100 g sln (compiler) ^a	$10^6 x_1$ (compiler) ^a
15	4.98 ± 0.19	5.99	8.97
25	5.20 ± 0.32	6.27	9.40
35	5.97 ± 0.41	7.22	10.8
45	7.02 ± 0.19	8.52	12.8
a Assuming s	cemperature (ref 1).		
	cemperature (ref 1).	INFORMATION	
The same to METHOD/APPARATUS/ The apparatus earlier design described in co 100-200 cm ³ of liquid (1) wen	cemperature (ref 1).	INFORMATION SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In stated purity, u further purifica (2) Redistilled; no	ent grade (Wako nd. Ltd.), no ased without ation.
The same to METHOD/APPARATUS/ The apparatus earlier design described in c 100-200 cm ³ of liquid (1) wer but connected After thermal lished a recin was used to va to transport to containing (2) were withdrawn	AUXILIARY /PROCEDURE: is similar to an h (ref 2) and is letail in the paper. (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- culating stream of air aporize liquid (1) and the vapor to the flask . Five 10 cm ³ aliquots h into separatory	SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In stated purity, u further purifica	ent grade (Wako nd. Ltd.), no ased without ation.
The same to METHOD/APPARATUS/ The apparatus earlier design described in of 100-200 cm ³ of liquid (1) wer but connected After thermal lished a recin was used to va to transport to containing (2) were withdrawn funnels. The (2) was then of into chlorofor spectrophotome	AUXILIARY /PROCEDURE: is similar to an h (ref 2) and is letail in the paper. (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- culating stream of air aporize liquid (1) and the vapor to the flask . Five 10 cm ³ aliquots	<pre>SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In stated purity, u further purifica (2) Redistilled; no given.  ESTIMATED ERROR: soly. see table, type specified. temp. ± 0.01°C.</pre>	ent grade (Wako nd. Ltd.), no used without ation. further details
The same to METHOD/APPARATUS/ The apparatus earlier design described in of 100-200 cm ³ of liquid (1) wer but connected After thermal lished a recin was used to va to transport to containing (2) were withdrawn funnels. The (2) was then of into chlorofor spectrophotome	AUXILIARY /PROCEDURE: is similar to an a (ref 2) and is letail in the paper. (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- culating stream of air aporize liquid (1) and the vapor to the flask . Five 10 cm ³ aliquots a liquots into separatory concentration of (1) in letermined by extraction rm followed by UV- etry. Standards for the etry were prepared by	SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In stated purity, u further purifica (2) Redistilled; no given. ESTIMATED ERROR: soly. see table, type specified.	ent grade (Wako nd. Ltd.), no used without ation. further details

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,3-Trimethylbenzene;	Sutton, C.; Calder, J.A.
C ₉ H ₁₂ ; [526-73-8]	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
(2) Artificial seawater (ref 1)	
VARIABLES: One temperature: 25.0°C	PREPARED BY:
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
one suffrity. S4.5 g suffs/kg sin	A. RICHSCHILL
EXPERIMENTAL VALUES:	
The solubility of 1,2,3-trimethylben	zene in artificial seawater is
reported to be 48.6 mg(1)/kg sln. T	he corresponding mass percent and
mole fraction, $x_1$ calculated by the	compiler are $4.86 \times 10^{-3} \text{ g(1)}/100 \text{ g}$
	ificial seawater composition of ref 1.
sin and 7.47 x 10 assuming the art	ciricial seawater composition of ref 1.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A test tube containing (1) was placed in a flask containing (2)	(1) from either Aldrich Chemical Co. or Matheson Coleman and
thus allowing for equilibration	Bell, 99+% pure.
through the vapor phase. The saturated solution was extracted	(2) made from doubly distilled
with hexane and analyzed by gas	water and salts 99+% pure.
chromatography.	
	ESTIMATED ERROR:
	temp. ± 0.1°C
1	soly. 0.5 (std. dev.)
	REFERENCES :
	1. Lyman, J.; Fleming, R.H.;
	J. Mar. Res. <u>1940</u> , 3, 135.
1	

COMPONENTS:	EVALUATOR:
<pre>(1) 1,2,4-Trimethylbenzene; C₉H₁₂; [95-63-6] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. August 1985.

Quantitative solubility data for 1,2,4-trimethylbenzene (1) in water (2) have been reported in the publications listed in Table 1.

## TABLE 1:Quantitative Solubility Studies of1,2,4-Trimethylbenzene(1) in Water

Reference	T/K	Method
McAuliffe (ref l)	298	GLC
Sutton and Calder (ref 2)	298	GLC
Price (ref 3)	298	GLC
Krzyzanowska and Szeliga (ref 4)	298	GLC
Sanemasa <i>et al</i> . (ref 5)	288-318	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data have been reported for the solubility of water in 1,2,4-trimethylbenzene.

All the available data are collected in Table 2 with the exception of that of Krzyzanowska and Szeliga (ref 4) which does not appear to be independent of that of Price (ref 3) and thus has been excluded from consideration. At 298K the only temperature where comparison is possible, the data are in excellent agreement so that the mean can be Recommended, although interestingly the value of Price (ref 3) is somewhat lower than those reported by other workers as for many of the higher hydrocarbons investigated by this author. At other temperatures only the data of Sanemasa *et al.* (ref 5) are available and must thus be regarded as Tentative.

TABLE	2:	Recommended								
		of 1,2,4-Tr	ime	thyll	benzene	(1)	in Wa	ter	(2)	

T/K	Solubility values					
	Reported values	"Best" values $(\pm \sigma_n)^{\alpha}$				
	10 ³ g(1)/100g sln	10 ³ g(l)/100g sln	¹⁰⁶ x1			
288	5.23 (ref 5)	5.2	7.8			
298	5.7 (ref 1), 5.90 (ref 2), 5.19 (ref 3), 5.65 (ref 5)	5.6 $\pm$ 0.3 (R)	8.4 (R)			
308	6.21 (ref 5)	6.2	9.3			
318	6.93 (ref 5)	6.9	10			

^α Obtained by averaging where appropriate; σ_n has no statistical significance. (continued next page)

COMPONENTS:EVALUATOR:(1) 1,2,4-Trimethylbenzene; C9H12;<br/>[95-63-6]G.T. Hefter, School of Mathematical<br/>and Physical Sciences, Murdoch<br/>University, Perth, W.A., Australia.<br/>August 1985

CRITICAL EVALUATION: (continued)

REFERENCES

1. McAuliffe, C. J. Phys. Chem. <u>1966</u>, 70, 1267-75.

- 2. Sutton, C.; Calder, J.A. J. Chem. Eng. Data <u>1975</u>, 20, 320-2.
- 3. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
- 4. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.
- 5. Sanemasa, I.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trimethylbenzene; C ₉ H ₁₂ ; [95-63-6]	McAuliffe, C.
	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES:	
	in untar at 2500 upg reported
The solubility of 1,2,4-trimethylben to be 57 $g(1)/10^6$ $g(2)$ .	Zene in water at 25°C was reported
The corresponding mass percent and m	ole fraction, $\pi_{-}$ calculated
by the compilers are 0.0057 g(1)/100	
by the complete are orotor, g(1,,	g bin and oto in ito
	i
	,
]	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	(1) Dhilling Datualoum on
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or	(1) Phillips Petroleum or Columbia Chemical; used
magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The	as received.
bottle was set aside for 2 days to	(2) distilled.
allow droplets of undissolved (1) to separate. Absence of emulsion	
was checked microscopically. A	
sample of the hydrocarbon-saturated water was withdrawn with a Hamilton	
syringe and gas liquid chromato-	HOMTHATED EDDAD-
graphed in conjunction with a flame- ionization detector.	temp. ± 1.5°C
	$soly. 4 g(1)/10^{6} g(2)$
	(standard deviation of mean)
	REFERENCES:
1	
1	

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COMPONENTS: (1) 1,2,4-Trimethylbenzene; C ₆ H ₁₂ ;	ORIGINAL MEASUREMENTS: Sutton, C.; Calder, J.A.
[95-63-6]	J. Chem. Eng. Data 1975, 20, 320-2.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of 1,2,4-trimethylben	
	onding mass percent and mole fraction,
$x_1$ , calculated by the compilers are	0.00590 g(l)/100 g sln and
$8.83 \times 10^{-6}$ .	
· ····	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	<ul> <li>(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.</li> </ul>
	(2) distilled.
	ESTIMATED ERROR:
[	temp. ± 0.1°C soly. 0.8 mg(1)/kg(2)
	(the standard deviation of the mean for six replicates)
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1,2,4-Trimethylbenzene; C₉H₁₂;</pre>	Price, L.C.
[95-63-6]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> ,
(2) Water; H ₂ O; [7732-18-5]	60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

## EXPERIMENTAL VALUES:

The solubility of 1,2,4-trimethylbenzene in water at 25°C and at system pressure was reported to be 51.9 mg(l)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 0.00519 g(l)/l00 g sln and 7.77 x 10⁻⁶.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de- tails are given in the paper.	<pre>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 1.2 mg(1)/kg(2) REFERENCES:</pre>		

```
COMPONENTS:

(1) 1,2,4-Trimethylbenzene; C<sub>9</sub>H<sub>12</sub>;

[95-63-6]

(2) Water; H<sub>2</sub>O; [7732-18-5]

VARIABLES:

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), <u>1978</u>, 12, 413-7.

PREPARED BY:
```

M.C. Haulait-Pirson

One temperature: 25°C

EXPERIMENTAL VALUES:

The solubility of 1,2,4-trimethylbenzene in water at  $25^{\circ}C$  was reported to be 51.9 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 0.00519 g(l)/100 g sln and 7.78 x  $10^{-6}$ .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways.	(1) not specified.
(2) were prepared in two ways. First, 200 $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	(2) not specified.
	ESTIMATED ERROR: soly. 1.6 mg(1)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES :

COMPONENTS:		ORIGIN	AL MEASUREMENTS:	
		Sanemasa, I.; Araki, M.;		
(1) 1,2,4-Trimethylbenzene; C ₉ H ₁₂ ;			chi, T.; Nagai, H.	
[95-63-6]				
(2) Water; H ₂ O; [77	32-18-5]	BULL.	Chem. Soc. Jpn. <u>198</u>	32, 55, 1054-62.
VARIABLES:		PREPAR	ED BY:	
Temperature: 15-45°	с		Hefter	
EXPERIMENTAL VALUES:				
	lubility of 1,2,4-t	rimet	hylbenzene in wate	er
$t/^{\circ}C$ 10 ⁴	mol(1)/dm ³ sln	1.03	$\pi(1)/(100) = \pi^{1}\pi^{1}$	1.06
	mol(1)/dm Sin		(compiler) ^a	$10^{6} x_{1}$
			(compiler)	(compiler) ^a
15	4.35 ± 0.12		5.23	7.84
25	4.69 ± 0.07		5.65	8.48
35	5.14 ± 0.20		6.21	9.32
45	5.71 ± 0.07		6.93	10.4
	AUXILIARY	INFORM	ATION	
METHOD/APPARATUS/PROCED	URE:	SOURCE	AND PURITY OF MATERI	ALS:
The apparatus is sin earlier design (ref described in detail 100-200 cm ³ of (2) a liquid (1) were place but connected thermon After thermal equili- lished a recirculati- was used to vaporize to transport the vap containing (2). Fiv were withdrawn into	2) and is in the paper. and 10-20 cm ³ of ced in separate ostatted flasks. brium was estab- ing stream of air a liquid (1) and bor to the flask ye 10 cm ³ aliquots	(1)	Analytical reagen Pure Chemical Ind purity 95.0%, use further purificat Redistilled; no f given.	. Ltd.), stated d without ion.
tunnels. The concer	stration of (1) in	ESTIM	ATED ERROR:	
(2) was then determined by extraction into chloroform followed by UV- spectrophotometry. Standards for the spectrophotometry were prepared by		soly. see table, type of error not specified. temp. ± 0.01°C.		
weight from pure lic	uid solutes.	REFER	ENCES :	
			ell, G.S. . Chem. Eng. Data <u>1</u>	<u>975</u> , 20, 97.
		ם ו	anemasa, I.; Arak eguchi, Y.; Nagai <i>hem. Lett.</i> <u>1981</u> , 2	, н.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trimethylbenzene;	Sutton, C.; Calder, J.A.
C ₉ H ₁₂ ; [95-63-6]	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
(2) Artificial seawater (ref l)	
VARIABLES:	PREPARED BY:
One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of 1,2,4-trimethylben	zene in artificial seawater is
reported to be 39.6 mg(l)/kg sln. T	he corresponding mass percent and
mole fraction, $x_1$ calculated by the	
sln and 6.09 x $10^{-6}$ assuming the art	ificial seawater composition of ref 1.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A test tube containing (1) was placed in a flask containing (2)	(1) from either Aldrich Chemical
thus allowing for equilibration	Co. or Matheson Coleman and Bell, 99+% pure.
through the vapor phase. The saturated solution was extracted	(2) mode from doubly distilled
with hexane and analyzed by gas	(2) made from doubly distilled water and salts 99+% pure.
chromatography.	
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.5 (std. dev.)
	REFERENCES :
	1. Lyman, J.; Fleming, R.H.;
	J. Mar. Res. <u>1940</u> , 3, 135.
1	
1	1

COMPONENTS:	EVALUATOR:
(1) Mesitylene; C ₉ H ₁₂ ; [108-67-8] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. August 1985

Quantitative solubility data for the mesitylene (1) - water (2) system have reported in the publications listed in Table 1.

	the second s	olubility Studie ater (2) System	es of
the Mesity	<u>rene (1) - w</u>	acer (2) bystem	
REFERENCE	T/K	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	residue volume
Andrews and Keefer (ref 2)	298	(1) in (2)	spectrophotometric
Guseva and Parnov (ref 3)	391-484	(1) in (2)	unspecified
Englin <i>et al</i> . (ref 4)	293-313	(2) in (1)	analytical
Sutton and Calder (ref 5)	298	(1) in (2)	GLC
Sanemasa $et al.$ (ref 6)	288-318	(1) in (2)	spectrophotometric
Sanemasa $et al.$ (ref 7)	288-318	(1) in (2)	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. THE SOLUBILITY OF MESITYLENE (1) IN WATER (2)

All the available data on the solubility of mesitylene in water at low temperatures (288-318K) are summarized in Table 2, except for the rejected values referred to below.

At 298K, the only temperature where comparison is possible, the datum of Sutton and Calder (ref 5) is in good agreement with the values reported by Sanemasa *et al.* (ref 6,7) enabling the mean to be Recommended. The datum of Andrews and Keefer (ref 2) is markedly higher than the other studies (ref 5,6,7) and is rejected as is the approximate value of Booth and Everson (ref 1).

At other temperatures only the two data sets of Sanemasa  $et \ al$ . (ref 6,7) are available and must thus be considered as Tentative.

At the elevated temperatures (*ca.* 390-480K) and system pressure only the data of Guseva and Parnov (ref 3) are available and thus no Critical Evaluation is possible. However, it may be noted that solubilities reported by Guseva and Parnov are not always reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

(continued next page)

COMPONENTS :	EVALUATOR:
<pre>(1) Mesitylene; C₉H₁₂; [108-67-8] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	August 1985.

 TABLE 2:
 Recommended (R) and Tentative Values of the Solubility

 of Mesitylene (1) in Water (2)

T/K	Solubility	y values .	
	Reported values	"Best" values (±	
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln l	.0 ⁶ x _l
288	4.56 (ref 6), 4.60 (ref 7)		.9
298	4.82 (ref 5), 4.95 (ref 6) 5.00 (ref 7)	$4.89 \pm 0.08^{a}(R)$ 7	.4 (R)
308	5.42 (ref 6), 5.49 (ref 7)	5.4 8	.2
318	5.65 (ref 6), 5.89 (ref 7)	5.7 8	.7

a Obtained by simple averaging;  $\sigma_n$  has no statistical significance.

## 2. THE SOLUBILITY OF WATER (2) IN MESITYLENE (1)

The solubility of water in mesitylene has been reported only by Englin  $et \ al$ . (ref 4) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for experimental values. However, it may be noted that for other hydrocarbon systems studies by Englin  $et \ al$ . their results are generally reliable at T < 300K but are higher than Recommended values at higher temperatures.

### REFERENCES

1.	Booth, H.S.; Everson, H.E. Ind. Eng. Chem. 1948, 40, 1491-3.
2.	Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
3.	Guseva, A.N.; Parnov, E.I. Vestn. Mosk. Univ. Khim. 1963, 18, 76-9.
4.	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
5.	Sutton, C.; Calder, J.A. J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
6.	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Chem. Lett. <u>1981</u> , 225-8.
7.	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 1982, 55, 1054-62.
8.	Alwani, Z.; Schneider, G.M. Ber. Bunsenges. Phys. Chem. <u>1969</u> , 73, 294-301.
NOTE	ADDED IN PROOF
Alwan	i and Schneider (ref 8) have also reported a critical locus of the
mesit	ylene-water system.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C ₉ H ₁₂ ; [108-67-8]	Booth, H.S.; Everson, H.E.
	Ind. Eng. Chem. 1948, 40, 1491-3.
(2) Water; H ₂ O; [7732-18-5]	inu: Eng. chem. <u>1940</u> , 10, 1491 5.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of mesitylene in wate	r at 25°C
was reported to be less than 0.02 g(	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Stanpared Pahaask tubog with neak	(1) course not creatified.
Stoppered Babcock tubes with neck graduated from 0 to 1.6 mL in steps	(1) source not specified; CP or highest commercial
of 0.02 mL were used. A known	grade; used as received.
volume of (2) (generally 50 mL)	
was added to the tube in a constant- temperature water bath and weighed	(2) distilled.
quantities of (1) were added to	
this solution. The mixture was	
then shaken for 5 minutes, returned	
to the bath for a minimum of 10 minutes and then centrifuged for	
5 minutes. After this treatment,	
the volume of residue was determined	ESTIMATED ERROR:
directly.	
	soly. ± 0.1 mL(1)/100 mL(2).
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C ₉ H ₁₂ ; [108-67-8] (2) Water; H ₂ O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. <i>J. Am. Chem. Soc.</i> <u>1950</u> , <i>72</i> , 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of mesitylene in wate to be 0.0097 g(l)/100 g sln. The corresponding mole fraction, $x_1$ , is 1.45 x 10 ⁻⁵ .	
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophoto- meter.	<ul> <li>(1) Eastman Kodak Co. white label; fractionally distilled; b.p. 165.0°C.</li> <li>(2) not specified.</li> </ul>
	not specified.
	-
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C ₉ H ₁₂ ; [108-67-8]	Guseva, A.N.; Parnov, E.I.
(2) Water; H ₂ O; [7732-18-5]	Vestn. Mosk. Univ. Khim. <u>1963</u> , 18, 76-9.
VARIABLES:	PREPARED BY:
Temperature: 118-211°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of me	esitylene in water
<i>t/°C</i> g(l)/100 g	$\frac{10^4 x_1}{(\text{compiler})}$
1180.0071440.0131870.0412110.078	0.10 0.19 0.61 1.17
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made in sealed glass tubes. No details	
were reported in the paper.	<pre>(1) source not specified;</pre>
	$n_D^{20}$ 1.49945.
	n _D ²⁰ 1.49945. (2) doubly distilled.
	n _D ²⁰ 1.49945. (2) doubly distilled. ESTIMATED ERROR:
	n _D ²⁰ 1.49945. (2) doubly distilled. ESTIMATED ERROR: not specified.
	n _D ²⁰ 1.49945. (2) doubly distilled. ESTIMATED ERROR: not specified.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C ₉ H ₁₂ ; [108-67-8] (2) Water· H ₂ O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-40°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Wat	er in Mestitylene
<u>t/°C</u> <u>g(2)/100 g sl</u>	$\frac{10^3 x_2 (\text{compiler})}{10^3 x_2 (\text{compiler})}$
20 0.0291 30 0.0393	1.94 2.62
40 0.0519	3.45
	х.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(1) Not specified.
for 5 hr. with (2). Next, calcium hydride was added and the evolving	(2) Not specified.
hydrogen volume measured and hence	
the concentration of (2) in (1) was	
evaluated.	
}	ESTIMATED ERROR:
	Not specified.
	DEFEDENCIC.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C ₉ H ₁₂ ; [108-67-8]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of mesitylene in wates	r at 25°C was reported to be
48.2 mg(1)/kg(2). The corresponding	mass percent and mole fraction,
$x_1$ , calculated by the compilers are (	).00482 g(l)/100 g sln and
$7.22 \times 10^{-6}$ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	<ul> <li>(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.</li> </ul>
	(2) distilled.
	ESTIMATED ERROR: temp. ± 0.1°C
	soly. 0.3 (the standard deviation of the mean for six replicates).
	REFERENCES :

COMPONENTS	:		ORIGINAL MEASUREMENTS	:
		9 ^H 12; [108-67-8]	Sanemasa, I.; Aral Nagai, H.	ki, M.; Deguchi, T.;
(2) Wate	r; H ₂ O; [	7732-18-5]	Chem. Lett. <u>1981</u>	, 225-8.
VARIABLES:			PREPARED BY:	
Temperat	ure: 15-4	5°C	M.C. Haulait-Pirso	on
EXPERIMENT	AL VALUES:			
		Solubility of mes	itylene in water	
	t/°C	g(l)/L	g(1)/100 g sln ^a	$\frac{10^6 x_1^{a}}{10^6 x_1^{a}}$
	15	0.0456 ± 0.0010	0.00456	6.82
	25	0.0495 ± 0.0015	0.00495	7.41
	35	0.0542 ± 0.0033	0.00542	8.11
	45	0.0565 ± 0.0031	0.00565	8.46
		AUXILIARY	INFORMATION	
	PARATUS / PRO	CEDURE :	SOURCE AND PURITY OF	
The appa	ratus use	CEDURE: d for attaining	SOURCE AND PURITY OF (1) analytical rea	MATERIALS: agent grade used as
The appa solubili in detai and redi	ratus use ty equili l in the stilled (	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a	SOURCE AND PURITY OF	
The appa solubili in detai and redi vessel a	ratus use ty equili l in the stilled ( nd a ther	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled.	
The appa solubili in detai and redi vessel a respecti erated b	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled.	
The appa solubili in detai and redi vessel a respecti erated b liquid s funnel a	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was nd circul	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled.	
The appa solubili in detai and redi vessel a respecti erated b liquid s funnel a pump. T	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was nd circul he circul	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a ation rate was 2 L/	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled.	
The appa solubili in detai and redi vessel a respecti erated b liquid s funnel a pump. T min. So attained	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was he circul he circul lubility within 5	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a ation rate was 2 L/ equilibria were min. Then portions	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled.	
The appa solubili in detai and redi vessel a respecti erated b liquid s funnel a pump. T min. So attained of 10 mL transfer	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was nd circul he circul lubility within 5 of the a red into	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a ation rate was 2 L/ equilibria were min. Then portions queous sln were funnels to which 10	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled. ESTIMATED ERROR:	agent grade used as
The appa solubili in detai and redi vessel a respecti erated b liquid s funnel a funnel a funnel a funnel of transfer mL of ch	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was nd circul he circul lubility within 5 of the a red into loroform	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a ation rate was 2 L/ equilibria were min. Then portions queous sln were funnels to which 10 had been added.	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled.	agent grade used as
The appa solubili in detai and redi vessel a respecti erated b liquid s funnel a pump. T min. So attained of 10 mL transfer mL of ch Experime spectrop	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was nd circul he circul lubility within 5 of the a red into loroform ntal proc hotometri	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a ation rate was 2 L/ equilibria were min. Then portions queous sln were funnels to which 10 had been added. edures involved in c measuring the	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled. ESTIMATED ERROR: soly. : given above	agent grade used as
The appa solubili in detai and redi vessel a respecti- erated b liquid s funnel a pump. T min. So attained of 10 mL transfer mL of ch Experime spectrop chlorofo	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was nd circul he circul lubility within 5 of the a red into loroform ntal proc hotometri rm extrac	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a ation rate was 2 L/ equilibria were min. Then portions queous sln were funnels to which 10 had been added. edures involved in	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled. ESTIMATED ERROR: soly. : given above	agent grade used as
The appa solubili in detai and redi vessel a respecti erated b liquid s funnel a pump. T min. So attained of 10 mL transfer mL of ch Experime spectrop chlorofo The solu that the	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was nd circul he circul lubility within 5 of the a red into loroform ntal proc hotometri rm extrac bility ru temperat	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a ation rate was 2 L/ equilibria were min. Then portions queous sln were funnels to which 10 had been added. edures involved in c measuring the ts were not reported ns were made such ure of solute reser-	SOURCE AND PURITY OF (1) analytical rea purchased. (2) redistilled. ESTIMATED ERROR: soly. : given above REFERENCES:	agent grade used as
The appa solubili in detai and redi vessel a respecti erated b liquid s funnel a pump. T min. So attained of 10 mL transfer mL of ch Experime spectrop chlorofo The solu that the voir was solvent	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was nd circul lubility within 5 of the a red into loroform ntal proc hotometri rm extrac bility ru temperat made to phase was	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a ation rate was 2 L/ equilibria were min. Then portions queous sln were funnels to which 10 had been added. edures involved in c measuring the ts were not reported ns were made such ure of solute reser- vary while that of held constant. The	SOURCE AND PURITY OF (1) analytical reapurchased. (2) redistilled. ESTIMATED ERROR: soly. : given above REFERENCES:	agent grade used as
The appa solubili in detai and redi vessel a respecti erated b liquid s funnel a pump. T min. So attained of 10 mL transfer mL of ch Experime spectrop chlorofo The solu that the voir was solvent solubili	ratus use ty equili l in the stilled ( nd a ther vely. Th y bubblin olute was nd circul he circul lubility within 5 of the a red into loroform ntal proc hotometri rm extrac bility ru temperat made to phase was ty obeys	CEDURE: d for attaining brium is described paper. Liquid (1) 2) were placed in a mostatted funnel e solute vapor, gen- g air through the introduced into the ated by means of a ation rate was 2 L/ equilibria were min. Then portions queous sln were funnels to which 10 had been added. edures involved in c measuring the ts were not reported ns were made such ure of solute reser- vary while that of	SOURCE AND PURITY OF (1) analytical reapurchased. (2) redistilled. ESTIMATED ERROR: soly. : given above REFERENCES:	agent grade used as

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Mesituler	e (1,3,5-Trimethyl-	Sanemasa, I.; Araki,	М.;
	C ₉ H ₁₂ ; [108-67-8]	Deguchi, T.; Nagai, H	H.
	0; [7732-18-5]	Bull. Chem. Soc. Jpn. 19	<u>982, 55,</u> 1054-62.
(1) #40017 #2	0, [,,52 10 0]		
VARIABLES:		PREPARED BY:	
Temperature:	15-45°C	G.T. Hefter	
EXPERIMENTAL VALU	UES:	<u> </u>	
r	The solubility of 1,3,5-t	rimethylbenzene in wat	er
t ∕°C	$10^4$ mol(1)/dm ³ sln	$10^3 \sigma(1)/100 \sigma cm$	$10^{6} x_{1}$
	10 mor(1)/dm sin	(compiler) ^a	÷
		(compiler)	(compiler) ^a
15	3.83 ± 0.15	4.60	6.90
25	4.15 ± 0.22	5.00	7.50
35	4.55 ± 0.23	5.49	8.22
45	4.85 ± 0.32	5.89	8.83
a Assuming a the same t			
	-	INFORMATION	
	AUXILIARY	INFORMATION SOURCE AND PURITY OF MATER	IALS :
the same the	AUXILIARY /PROCEDURE:	SOURCE AND PURITY OF MATER	
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper.	SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us	ent grade (Wako d. Ltd.), stated ed without
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of	SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In	ent grade (Wako d. Ltd.), stated ed without
The same for the s	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks.	SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us	ent grade (Wako d. Ltd.), stated ed without ttion.
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab-	SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica	ent grade (Wako d. Ltd.), stated ed without tion.
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- rculating stream of air aporize liquid (1) and	<ul> <li>SOURCE AND PURITY OF MATER</li> <li>(1) Analytical reage Pure Chemical In purity 97.0%, us further purifica</li> <li>(2) Redistilled; no</li> </ul>	ent grade (Wako d. Ltd.), stated ed without tion.
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- rculating stream of air aporize liquid (1) and the vapor to the flask	<ul> <li>SOURCE AND PURITY OF MATER</li> <li>(1) Analytical reage Pure Chemical In purity 97.0%, us further purifica</li> <li>(2) Redistilled; no given.</li> </ul>	ent grade (Wako d. Ltd.), stated ed without ttion.
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- rculating stream of air aporize liquid (1) and	<ul> <li>SOURCE AND PURITY OF MATER</li> <li>(1) Analytical reage Pure Chemical In purity 97.0%, us further purifica</li> <li>(2) Redistilled; no given.</li> </ul>	ent grade (Wako d. Ltd.), stated ed without ttion.
The same of the sa	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- rculating stream of air aporize liquid (1) and the vapor to the flask ). Five 10 cm ³ aliquots n into separatory concentration of (1) in	<ul> <li>SOURCE AND PURITY OF MATER</li> <li>(1) Analytical reage Pure Chemical In purity 97.0%, us further purifica</li> <li>(2) Redistilled; no given.</li> </ul>	ent grade (Wako ad. Ltd.), stated aed without ation. further details
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- rculating stream of air aporize liquid (1) and the vapor to the flask ). Five 10 cm ³ aliquots n into separatory concentration of (1) in determined by extraction rm followed by UV- etry. Standards for the	<ul> <li>SOURCE AND PURITY OF MATER</li> <li>(1) Analytical reage Pure Chemical In purity 97.0%, us further purifica</li> <li>(2) Redistilled; no given.</li> </ul>	ent grade (Wako ad. Ltd.), stated aed without ation. further details
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- rculating stream of air aporize liquid (1) and the vapor to the flask ). Five 10 cm ³ aliquots n into separatory concentration of (1) in determined by extraction rm followed by UV- etry. Standards for the etry were prepared by	<ul> <li>SOURCE AND PURITY OF MATER</li> <li>(1) Analytical reage Pure Chemical In purity 97.0%, us further purifica</li> <li>(2) Redistilled; no given.</li> </ul>	ent grade (Wako ad. Ltd.), stated aed without ation. further details
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- rculating stream of air aporize liquid (1) and the vapor to the flask ). Five 10 cm ³ aliquots n into separatory concentration of (1) in determined by extraction rm followed by UV- etry. Standards for the	<pre>SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no given.  ESTIMATED ERROR: soly. see table, type specified: temp. ± 0.1°C.</pre>	ent grade (Wako d. Ltd.), stated ed without tion. further details
the same the	AUXILIARY /PROCEDURE: is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- rculating stream of air aporize liquid (1) and the vapor to the flask ). Five 10 cm ³ aliquots n into separatory concentration of (1) in determined by extraction rm followed by UV- etry. Standards for the etry were prepared by	<pre>SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no given.  ESTIMATED ERROR: soly. see table, type specified. temp. ± 0.1°C. REFERENCES: 1. Kell, G.S.</pre>	ent grade (Wako d. Ltd.), stated ed without tion. further details of error not <u>1975</u> , 20, 97.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene (1,3,5-Trimethyl-	Sutton, C.; Calder, J.A.
benzene); $C_{9}H_{12}$ ; [108-67-8]	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
(2) Artificial seawater (ref l)	
VARIABLES:	PREPARED BY:
One temperature: 25.0°C	
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of 1,3,5-trimethylben:	zene in artificial seawater is
reported to be 31.3 mg(l)/kg sln. Th	
mole fraction, $x_1$ calculated by the c	
sln and 4.81 x $10^{-6}$ assuming the article	ificial seawater composition of ref 1.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A test tube containing (1) was	(1) from either Aldrich Chemical
placed in a flask containing (2)	Co. or Matheson Coleman and Bell, 99+% pure.
thus allowing for equilibration through the vapor phase. The	
saturated solution was extracted with hexane and analyzed by gas	(2) made from doubly distilled water and salts 99+% pure.
chromatography.	
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.2 (std. dev.)
	REFERENCES:
	1. Lyman, J.; Fleming, R.H.;
	J. Mar. Res. <u>1940</u> , 3, 135.

COMPONENTS :	EVALUATOR:
<pre>(1) Cumene; C₉H₁₂; [98-82-8] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986.

Quantitative solubility studies of the cumene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of

Reference	T/K	Solubility	Method
Stearns et al. (ref 1)	298	(l) in (2)	turbidimetric
Andrews and Keefer (ref 2)	298	(1) in (2)	spectrophotometric
Glew and Robertson (ref 3)	298-354	(1) in (2)	spectrophotometric
McAuliffe (ref 4)	298	(l) in (2)	GLC
Englin <i>et al</i> . (ref 5)	273-323	(2) in (1)	analytical
McAuliffe (ref 6)	298	(1) in (2)	GLC
Sutton and Calder (ref 7)	298	(l) in (2)	GLC
Price (ref 8)	298	(l) in (2)	GLC
Krzyzanowska and Szeliga (ref 9)	298	(1) in (2)	GLC
Sanemasa $et al.$ (ref 10)	288-318	(1) in (2)	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

#### 1. THE SOLUBILITY OF CUMENE (1) IN WATER (2)

With the exception of the rejected values referred to below and the datum of Krzyzanowska and Szeliga (ref 9) which does not appear to be independent of that of Price (ref 8) all the available data on the solubility of cumene in water are summarized in Table 2.

At 298K where the most data are available, agreement is only fair. The values of Stearns *et al.* (ref 1), Andrews and Keefer (ref 2) and Glew and Robertson (ref 3) are much higher than other studies (ref 4,6,7,8,10) and are rejected.

At other temperatures the values of Glew and Robertson are again in only fair agreement with those of Sanemasa  $et \ al$ . (ref 10), but in the absence of confirmatory studies it is not possible to express a preference for either data set, and the averaged "Best" values should be regarded as Tentative. Selected data are also plotted in Figure 1

(continued next page)

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COMPONENTS:

(1) Cumene; C<sub>9</sub>H<sub>12</sub>; [98-82-8]

(2) Water; H<sub>2</sub>O; [7732-18-5]

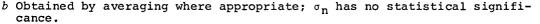
University, Perth, W.A., Australia.

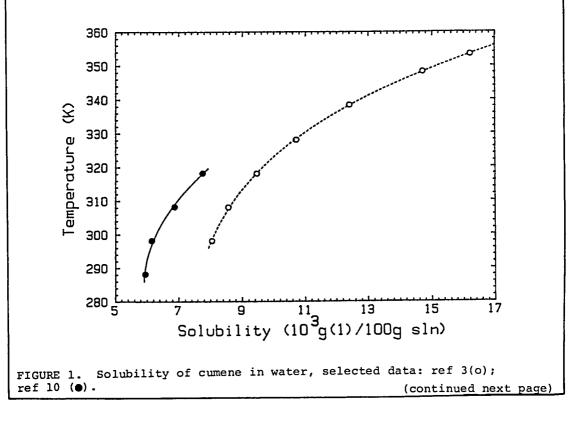
January 1986.
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TABLE 2:	Tentative	Values of	E the	Solubility	of
	Cumene (1	) in Water	c (2)		

T/K	Solubility	values ·	
	Reported values ^a	"Best" values	$(\pm \sigma_n)^b$
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln	10 ⁵ x ₁
288	5.95 (ref 10)	6.0	0.90
298	5.3 (ref 4), 5.0 (ref 6), 6.53 (ref 7), 4.83 (ref 8), 6.15 (ref 10)	5.6 ± 0.7	0.84
303	8.3* (ref 3), 6.5* (ref 10)	7.4 ± 0.9	1.11
313	9.0* (ref 3), 7.3* (ref 10)	8.2 ± 0.9	1.23
323	10.0* (ref 3), 8.0* (ref 10)	9 ± 1	1.3
333	11.5* (ref 3)	12	1.8
343	13.5* (ref 3)	14	2.1
353	16.1* (ref 3)	16	2.4

*a* Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.





COMPONENTS:	EVALUATOR:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

Interestingly, application of the van't Hoff equation to both data sets gives values of  $\Delta H_{sln} = 3.5$  (ref 3) and 5.1 (ref 10) kJ mol⁻¹ and  $\Delta C_{p,sln} = 291$  (ref 3) and 382 (ref 10) J K⁻¹ mol⁻¹. Comparison of these values with those of related systems suggests both solubility data sets are reasonable.

2. THE SOLUBILITY OF WATER (2) IN CUMENE (1)

Quantitative solubilities of water in cumene have been reported only in the study of Englin *et al.* (ref 5) and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet following this Critical Evaluation for the experimental values. However, it may be noted that for other hydrocarbon systems studied by these authors, the data of Englin *et al.* are generally reliable at T < 300K but higher than Recommended values at higher temperatures.

#### REFERENCES

- Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkin, L.D. J. Chem. Phys. <u>1947</u>, 15, 496-507.
- 2. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1950, 72, 5034-7.
- 3. Glew, D.N.; Robertson, R.E. J. Phys. Chem. <u>1956</u>, 60, 332-7.
- 4. McAuliffe, C. Nature 1963, 200, 1092-3.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1966</u>, 10, 1267-75.
- 6. McAuliffe, C. J. Phys. Chem. 1966, 70, 1267-75.
- 7. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.
- 8. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
- 9. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.
- 10. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62.

### ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for graphics and regression analyses.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8] (2) Water; H ₂ O; [7732-18-5]	<pre>Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D. J. Chem. Phys. <u>1947</u>, 15, 496-507.</pre>
VARIABLES: Temperature: 25°C	PREPARED BY: A. Maczynski and D. Shaw
EXPERIMENTAL VALUES: The solubility of cumene in water at 0.017 g(1)/100 g sln. The corresponding mole fraction, $x_1$ , is 2.5 x 10 ⁻⁵ .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE: Mixtures of (1) in (2) of known composition were shaken for at least 48 hours. The turbidity was then measured with a photo- meter. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.
	ESTIMATED ERROR: temp. ± 3°C. REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ 0; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	L
The solubility of cumene in water at to be 0.0073 g(1)/100 g sln. The corresponding mole fraction, $x_1$ , is 1.09 x 10 ⁻⁵ .	
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank	<ul> <li>(1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 151.5-152.0°C.</li> <li>(2) not specified.</li> </ul>
On the Beckman spectrophotometer.	ESTIMATED ERROR:
	not specified.
	REFERENCES:
l	

COMPONENTS:			ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H	H12; [98-82-8	3]	Glew, D.N.; Robertson, R.E.
(2) Water; H ₂ O;			J. Phys. Chem. <u>1956</u> , 60, 332-7.
VARIABLES:	·····-		PREPARED BY:
			FREFARED BY:
Temperature: 2			A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES	3:		
	Solu	bility of	cumene in water
	т/к	$\frac{10^5 x_1}{10^5 x_1}$	g(l)/100 g sln (compiler)
-	298.086 303.134 308.068 313.108 318.055 323.052 328.066 333.133 338.315 343.470 348.247 353.359	1.2050 1.2416 1.2825 1.3446 1.4162 1.5037 1.6011 1.7221 1.8624 2.0302 2.2064 2.4212	0.00804 0.00829 0.00856 0.00897 0.00945 0.01004 0.01069 0.01149 0.01243 0.01355 0.01472 0.01616
		AUXILIARY	INFORMATION
METHOD/APPARATUS/PI	ROCEDURE :		SOURCE AND PURITY OF MATERIALS:
Component (1) w surface of the water and the a pumped steadily through the qua where its absor From these valu of (1) in (2) w	main body of queous solut in a closed rtz absorpti bance was me es the solub	the ion was circuit on cell asured. ility	<ul> <li>(1) Eastman Kodak Co. White Label; distilled in an atmosphere of nitrogen; b.p.range 0.2°C, passed repeatedly through a fresh column of Fisher activated alumina,</li> <li>(2) distilled; passed through a demineralizing column.</li> </ul> ESTIMATED ERROR: temp. ± 0.002 K soly. ± 1.00% at 25°C and ± 1.25% at 80°C (standard error) REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) <u>1963</u> , 200, 1092-3.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of cumene in water at	25°C was reported
to be 0.0053 g(1)/100 g sln.	calculated by the compilers
The corresponding mole fraction, $x_1$ , is 7.9 x 10 ⁻⁶ .	calculated by the compliers
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The saturated solution of (1) in	(1) Phillips Petroleum Co.; 99+%;
(2) was prepared by either shaking vigorously on a reciprocal shaker	used as received.
Or stirring for several days with a magnetic stirrer.	(2) distilled.
A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was	
injected directly into a gas liquid	
chromatograph.	
	ESTIMATED ERROR:
	temp. ± 1.5°C
	soly. 0.0005 (standard deviation of mean)
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel 1965,
	10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 0-50°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of W	Mater in Cumene .
<i>t/°C</i> g(2)/100 g sln	$10^3 x_2$ (compiler)
0 0.0156	1.04
10 0.0219 20 0.0303	1.46 2.02
30 0.0407 40 0.0550	2.71 3.66
50 0.0710	4.72
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hr. with (2). Next, calcium	(2) Not specified.
hydride was added and the evolving hydrogen volume measured and hence	
the concentration of (2) in (1) was	
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

195
ORIGINAL MEASUREMENTS:
McAuliffe, C.
J. Phys. Chem. <u>1966</u> , 70, 1267-75.
PREPARED BY: A. Maczynski, Z. Maczynska, and
A. Szafranski
25°C was reported ole fraction, $x_1$ , calculated g sln and 7.5 x $10^{-6}$ .
INFORMATION
SOURCE AND PURITY OF MATERIALS:
<pre>(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 5 g(1)/10⁶ g(2) (standard deviation of mean) REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	L
The solubility of cumene in water at	25°C was reported to be
65.3 mg(1)/kg(2). The corresponding	mass percent and mole fraction,
$x_1$ , calculated by the compilers are	0.00653 g(l)/100 g sln and
9.78 x $10^{-6}$ .	
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
	(2) distilled.
	ESTIMATED ERROR: temp. ± 0.1°C
	soly. 0.8 (the standard deviation of the mean for six replicates)
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Ат. Аввос. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

# EXPERIMENTAL VALUES:

The solubility of cumene in water at 25°C and at system pressure was reported to be 48.3 mg(l)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 0.00483 g(l)/l00 g sln and 7.23 x  $10^{-6}$ .

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de- tails are given in the paper.	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>(2) distilled.</li> </ul>	
	ESTIMATED ERROR: temp. ± 1°C soly. ± 1.2 mg(1)/kg(2)	
	REFERENCES :	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Krzyzanowska, T.; Szeliga, J.	
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.	
	<i>hajba (habbabbe)</i> , <u>1570</u> , 15, 415 /.	
VARIABLES:	PREPARED BY:	
	I REFARED BI:	
One temperature: 25°C	M.C. Haulait-Pirson	
	·	
EXPERIMENTAL VALUES:		
The solubility of cumene in water at	25°C was reported	
to be 48.3 mg(1)/kg(2).		
The corresponding made percent and me	le fraction a coloulated	
The corresponding mass percent and mo	- ,	
by compiler are 0.00483 g(l)/100 g sl	n and 7.24 x $10^{-6}$ .	
Editor's Note: Based on the results		
systems, uncertainity exists about whether the datum compiled here is		
independent of that of Price for the		
independent of that of Price for the		
independent of that of Price for the	same system (see previous page).	
independent of that of Price for the AUXILIARY	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS:	
independent of that of Price for the AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways.	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified.	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS:	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1)	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified.	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat-	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR:	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	<pre>same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: soly. 1.44 mg(1)/kg(2) (standard</pre>	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat-	same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR:	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	<pre>same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: soly. 1.44 mg(1)/kg(2) (standard</pre>	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	<pre>same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: soly. 1.44 mg(1)/kg(2) (standard deviation from 7-9 determinations).</pre>	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	<pre>same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: soly. 1.44 mg(1)/kg(2) (standard deviation from 7-9 determinations).</pre>	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	<pre>same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: soly. 1.44 mg(1)/kg(2) (standard deviation from 7-9 determinations).</pre>	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	<pre>same system (see previous page). INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: soly. 1.44 mg(1)/kg(2) (standard deviation from 7-9 determinations).</pre>	

COMPONENTS :		ORIGINAL MEASUREMENTS:	
(1) Cumene (Isopropylbenzene); C ₉ H ₁₂ ;		Sanemasa, I.; Araki, M. Deguchi, T.; Nagai, H.	,
[98-82-8]		Bull. Chem. Soc. Jpn. <u>1982</u> , 55, 1054-6	
(2) Water; H ₂ O; [7732-18-5]		<u></u>	
	1		:
VARIABLES:		PREPARED BY:	
Temperature: 15-45°C		G.T. Hefter	
EXPERIMENTAL VALUES:			
The solubility	of isop	ropylbenzene in water	
$t/^{\circ}C$ 10 ⁴ mol(1)/dm ³	sln	$10^3 g(1)/100 g sln$	$10^{6} x_{1}$
		(compiler) ^a	(compiler) ^a
15 4.95 ± 0.28	1	5,95	8.92
25 5.10 ± 0.45		6.15	9.22
35 5.68 ± 0.22	!	6.87	10.3
45 6.38 ± 0.24		7.75	11.6
			<u></u>
A	JXILIARY	INFORMATION	
METHOD / APPARATUS / PROCEDURE :	·	·····	
The apparatus is similar to an		SOURCE AND PURITY OF MATERIAN (1) Analytical reagent	
earlier design (ref 2) and is described in detail in the pape 100-200 cm ³ of (2) and 10-20 cm	³ of	Pure Chemical Ind. purity 98.0%, used further purification	Ltd.), stated without
liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots		(2) Redistilled; no fu given.	rther details
were withdrawn into separatory			
funnels. The concentration of (2) was then determined by extr		ESTIMATED ERROR:	f orror not
into chloroform followed by UV- spectrophotometry. Standards for the spectrophotometry were prepared by		<pre>soly. see table, type o specified. temp. ± 0.01°C.</pre>	I error not
weight from pure liquid solutes	•	REFERENCES :	
		1. Kell, G.S. J. Chem. Eng. Data <u>19</u>	<u>75</u> , 20, 97.
		<ol> <li>Sanemasa, I.; Araki Deguchi, Y.; Nagai, Chem. Lett. <u>1981</u>, 225</li> </ol>	н.
·····			

200		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Sutton, C.; Calder, J.A.	
(2) Artificial seawater (ref 1)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.	
VARIABLES: One temperature: 25.0°C	PREPARED BY:	
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt	
EXPERIMENTAL VALUES:		
The solubility of cumene (isopropylb	enzene) in artificial seawater is	
reported to be 42.5 mg(1)/kg sln. T		
mole fraction, $x_1$ calculated by the		
sln and 6.54 x $10^{-6}$ assuming the art		
ref 1.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration	<ul> <li>(1) from either Aldrich Chemical</li> <li>Co. or Matheson Coleman and</li> <li>Bell, 99+% pure.</li> </ul>	
through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas	(2) made from doubly distilled water and salts 99+% pure.	
chromatography.		
	ESTIMATED ERROR:	
	temp. ± 0.1°C	
	soly. 0.2 (std. dev.)	
	REFERENCES: 1. Lyman, J.; Fleming, R.H.;	
	J. Mar. Res. <u>1940</u> , 3, 135.	
1		

COMPONENTS:	EVALUATOR:
<pre>(1) Propylbenzene, C₉H₁₂; [103-65-1] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION:

Quantitative solubility data for propylbenzene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in propylbenzene.

# TABLE 1: Quantitative Solubility Studies ofPropylbenzene (1) in Water (2)

Reference	T/K	Method
Fühner (ref 1)	288	volumetric
Stearns et al. (ref 2)	298	turbidimetric
Andrews and Keefer (ref 3)	298	spectrophotometric
Klevens (ref 4)	298	spectrophotometric
Guseva and Parnov (ref 5)	359-495	synthetic
Krasnoshchekova and Gubergrits (ref 7)	298	GLC
Sanemasa $et \ al.$ (ref 8)	288-318	spectrophotometric
Sanemasa $et \ al.$ (ref 9)	298	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

Guseva and Parnov (ref 5) have reported solubility data for propylbenzene in water at elevated temperatures (359-495K) and system pressure. Alwani and Schneider (ref 6) have studied phase equilibria in the propylbenzene water system at 600-678K and 20-200 MPa. In the absence of confirmatory studies no Critical Evaluation of these data is possible; however, it may be noted that data reported by Guseva and Parnov (ref 5) for other hydrocarbon - water systems are generally not reliable. The interested user is referred to the relevant Data Sheets for experimental results.

All other data for the solubility of propylbenzene in water are summarized in Table 2 except for the 298K data of Fühner (ref 1) and Klevens (ref 4) which are very much higher than all other studies (ref 3,7,8,9) and are rejected. The remaining data at 298K, the only temperature where comparison is possible, are in only fair agreement.

At other temperatures only the values of Sanemasa  $et \ al$ . (ref 8) are available. Thus all solubility values in Table 2 must be considered Tentative.

(continued next page)

DNENTS:	EVALUATOR:	
2 20	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.	
	March 1986.	
CAL EVALUATION: (continued)	· · · · · · · · · · · · · · · · · · ·	
TABLE 2: Tentative Values of the Solubility of Propylbenzene (1) in Water (2)		
T/K Solubility values		
Reported values	"Best" values $(\pm \sigma_n)^a$	
10 ³ g(1)/100g sln	$10^{3}$ g(1)/100g sln $10^{6} x_{1}$	
4.66 (ref 8)	4.7 7.0	
5.5 (ref 3), 7.0 (ref 7) 5.10 (ref 8), 4.52 (ref 9)	5.5 ± 0.9 8.2	
5.50 (ref 8)	5.5 8.2	
6.41 (ref 8)	6.4 9.6	
ance.		
1. Fuhner, H. Chem. Ber. <u>1924</u> , 57, 510-4.		
2. Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, L.D. J. Chem. Phys. <u>1947</u> , 15, 496-507.		
3. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.		
4. Klevens, H.B. J. Phys. Chem. <u>1950</u> , 54, 283-98.		
5. Guseva, A.N.; Parnov, E.I. Zh. Fiz. Khim. <u>1964</u> , 38, 805-6.		
6. Alwani, Z.; Schneider, G.M. Ber. Bunsenges. Phys. Chem. <u>1969</u> , 73, 294-301.		
Krasnoshchekova, R.Y.; Gubergrit 170-3.	s, M.Y. Vodnye. Resursy. <u>1975</u> , 2,	
Sanemasa, I.; Araki, M.; Deguchi <u>1982</u> , <i>55</i> , 1054-62.	., T.; Nagai, J. Bull. Chem. Soc. Jpn.	
Sanemasa, I.; Arakawa, S.; Araki Jpn. <u>1984</u> , 57, 1539-44.	, M.; Deguchi, T. Bull. Chem. Soc.	
	Propylbenzene (           Sol           Reported values           10 ³ g(1)/100g sln           4.66 (ref 8)           5.5 (ref 3), 7.0 (ref 7)           5.50 (ref 8)           6.41 (ref 8)           Otained by averaging where appropriance.           ERENCES           Fuhner, H. Chem. Ber. 1924, 57           Stearns, R.S.; Oppenheimer, H.;           Phys. 1947, 15, 496-507.           Andrews, L.J.; Keefer, R.M. J.           Klevens, H.B. J. Phys. Chem. 1           Guseva, A.N.; Parnov, E.I. Zh.           Alwani, Z.; Schneider, G.M. Ber           294-301.           Krasnoshchekova, R.Y.; Gubergritt           170-3.           Sanemasa, I.; Araki, M.; Deguchi           1982, 55, 1054-62.           Sanemasa, I.; Arakawa, S.; Araki	

COMPONENTS :	CONTCINAL AMAGUNANTA
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C ₉ H ₁₂ ; [103-65-1]	Fuhner, H.
(2) Water; H ₂ O; [7732-18-5]	Ber. Dtsch. Chem. Ges. 1924, 57, 510-5.
VARIABLES:	PREPARED BY:
One temperature: 15°C	A. Maczynski, Z. Maczynska and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of propylbenzene in wa 0.006 g(1)/100 g sln. The corresponding mole fraction, $x_1$ , is 9 x 10 ⁻⁶ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 cm ³ (2) until a completely clear solution was no longer obtained at the experimental temperature.	<ul> <li>(1) source not specified; commercial grade; used as received,</li> <li>(2) not specified.</li> </ul>
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Propylbenzene; C9^H12; [103-65-1]</pre>	<pre>Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D.</pre>
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Phys. <u>1947</u> , 15, 496-507.
VARIABLES:	PREPARED BY:
Temperature: 25°C	A. Maczynski and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of propylbenzene in wa 0.012 g(l)/100 g sln.	
The corresponding mole fraction, $x_1$ , is 1.8 x 10 ⁻⁵ .	calculated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Mixtures of (1) in (2) of known	(1) not specified.
composition were shaken for at least 48 hours. The turbidity was then measured with a photo-	(2) not specified.
meter. Turbidities of several mixture compositions were plotted	
and the sharp break point taken as the solubility.	
the solubility.	
	ESTIMATED ERROR:
	temp. ± 3°C.
	REFERENCES:
	1

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Propylbenzene; C ₉ H ₁₂ ; [103-65-1]		
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
The solubility of propylbenzene in water at 25°C was reported to be 0.0055 g(1)/100 g sln. The corresponding mole fraction, $x_1$ , calculated by the compilers is 8.2 x 10 ⁻⁶ .		
AUXILIARY	INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorb- ance of the hexane phase was meas- ured against a hexane blank on the Beckman spectrophotometer.	<ul> <li>(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. range 157.8-158.1°C.</li> <li>(2) not specified.</li> </ul>	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C ₉ H ₁₂ ; [103-65-1]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
2	
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of propylbenzene in wa	
0.12 g(1) $L^{-1}$ sln and 0.001 mol(1)	L ⁻¹ sln.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was	(1) not specified.
determined by shaking small amounts of (1) in 1 liter of (2) for as long	(2) not specified.
as three months. Aliquots were removed and concentrations deter-	(2) not specified.
mined by spectra.	
	ESTIMATED EDDOD.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :
	NJE BABNGES ;
1	
1	1

COMPONENTS: (1) Propylbenzene; C ₉ H ₁₂ ; [103-65-1]	ORIGINAL MEASUREMENTS:
(2) Water; H ₂ O; [7732-18-5]	Zh. Fiz. Khim. <u>1964</u> , 38, 805-6.
VARIABLES:	PREPARED BY:
Temperature: 85.8-222.0°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of p	copylbenzene in water
<i>t/°C</i> g(l)/100 g	$\frac{10^5 x_1}{2}$ (compiler)
85.80.0132114.50.0166140.50.0323188.00.087222.00.245	5 2.49
	INFORMATION
METHOD/APPARATUS/PROCEDURE: The measurements were made in sealed glass tubes. No details	SOURCE AND PURITY OF MATERIALS: (1) not specified.
METHOD/APPARATUS/PROCEDURE: The measurements were made in	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: The measurements were made in sealed glass tubes. No details	SOURCE AND PURITY OF MATERIALS: (1) not specified.
METHOD/APPARATUS/PROCEDURE: The measurements were made in sealed glass tubes. No details	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.
METHOD/APPARATUS/PROCEDURE: The measurements were made in sealed glass tubes. No details	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR:
METHOD/APPARATUS/PROCEDURE: The measurements were made in sealed glass tubes. No details	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: not specified.

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COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Propylbenzene; C₉H₁₂; [103-65-1] (2) Water; H₂O; [7732-18-5]</pre>	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. <i>Vodnye. Resursy.</i> <u>1975</u> , 2, 170-3.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of propylbenzene in wa to be 0.070 mg(1) cm ⁻³ sln. The corresponding mass percent and mo by the compiler are 0.0070 g(1)/100 g assumption that 1.00 cm ⁻³ sln = 1.00	the fraction, $x_1$ , calculated sin and 1.05 x $10^{-5}$ . The
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc.	(1) described in ref (1).
A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G column operated at 90-140°C.	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 1°C
	REFERENCES:
	<pre>1. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya 1973, 13, 885.</pre>

COMPONENTS:		ORIGINAL	. MEASUREMENTS:	
(1) Propylbenzene; C ₉ H ₁	.: [103-65-1]	Sanema	asa, I.; Araki, M.	:
(2) Water; H ₂ O; [7732-1			hi, T.; Nagai, H.	
		-	Chem. Soc. Jpn. 1982	, 55, 1054-62.
			<u></u>	
VARIABLES:		PREPAREI	D BY:	
Temperature: 15-45°C		G.T. H	Hefter	
EXPERIMENTAL VALUES:			······································	
The se	olubility of pr	opylben	zene in water	
$t/^{\circ}$ C $10^4$ mol		1.3	(1) (1001-	6
t/0C 10 mol	(1)/dm ⁻ sin			$10^{6} x_{1}$
		(0	compiler) ^{<i>a</i>}	(compiler) ^a
15 3.8	8 ± 0.15	<u></u>	4.66	6.99
	$3 \pm 0.12$		5.10	7.64
	5 ± 0.07		5.50	8.25
	8 ± 0.17		6.41	9.61
a Assuming solution d the same temperatur		the sam	ne as those of pur	e water at
		the sam	ne as those of pur	e water at
	e (ref 1).			e water at
		INFORMAT		
the same temperatur	e (ref 1).	INFORMAT	TION AND PURITY OF MATERIAL	.5 :
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila	e (ref 1). AUXILIARY r to an	INFORMAT SOURCE A	TON AND PURITY OF MATERIAI Analytical reagent	.S: grade (Wako
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in	e (ref 1). AUXILIARY r to an and is the paper.	INFORMAT SOURCE A (1) P F S	TON AND PURITY OF MATERIAN Analytical reagent Pure Chemical Ind. Stated purity, used	.S: grade (Wako Ltd.), no l without
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and	e (ref 1). AUXILIARY r to an and is the paper. 10-20 cm ³ of	INFORMAT SOURCE A (1) P F S	TON AND PURITY OF MATERIAN Analytical reagent Pure Chemical Ind.	.S: grade (Wako Ltd.), no l without
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta	r to an and is the paper. 10-20 cm ³ of in separate tted flasks.	INFORMAT SOURCE A (1) P E S f (2) F	TION AND PURITY OF MATERIAL Analytical reagent Pure Chemical Ind. Stated purity, used Stated purity, used Stated purity, no fu	.S: grade (Wako Ltd.), no 1 without on.
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta After thermal equilibri	r to an and is the paper. 10-20 cm ³ of in separate tted flasks. um was estab-	INFORMAT SOURCE A (1) P E S f (2) F	TION AND PURITY OF MATERIAL Analytical reagent Pure Chemical Ind. Stated purity, used Further purificatio	.S: grade (Wako Ltd.), no 1 without on.
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta After thermal equilibri lished a recirculating was used to vaporize li	r to an and is the paper. 10-20 cm ³ of in separate tted flasks. um was estab- stream of air quid (1) and	INFORMAT SOURCE A (1) P E S f (2) F	TION AND PURITY OF MATERIAL Analytical reagent Pure Chemical Ind. Stated purity, used Stated purity, used Stated purity, no fu	.S: grade (Wako Ltd.), no 1 without on.
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta After thermal equilibri lished a recirculating was used to vaporize li to transport the vapor containing (2). Five 1	r to an and is the paper. 10-20 cm ³ of in separate tted flasks. um was estab- stream of air quid (1) and to the flask 0 cm ³ aliquots	INFORMAT SOURCE A (1) P E S f (2) F	TION AND PURITY OF MATERIAL Analytical reagent Pure Chemical Ind. Stated purity, used Stated purity, used Stated purity, no fu	.S: grade (Wako Ltd.), no 1 without on.
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta After thermal equilibri lished a recirculating was used to vaporize li to transport the vapor containing (2). Five 1	r to an and is the paper. 10-20 cm ³ of in separate tted flasks. um was estab- stream of air quid (1) and to the flask 0 cm ³ aliquots aratory	INFORMAT SOURCE A (1) P F S f (2) F S	TION AND PURITY OF MATERIAL Analytical reagent Pure Chemical Ind. Stated purity, used Stated purity, used Stated purity, no fu	.S: grade (Wako Ltd.), no 1 without on.
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta After thermal equilibri lished a recirculating Was used to vaporize li to transport the vapor containing (2). Five 1 were withdrawn into sep funnels. The concentra (2) was then determined	AUXILIARY r to an and is the paper. 10-20 cm ³ of in separate tted flasks. um was estab- stream of air quid (1) and to the flask 0 cm ³ aliquots aratory tion of (1) in by extraction	INFORMAT SOURCE A (1) P S f (2) F S S ESTIMAT	TION AND PURITY OF MATERIAL Pure Chemical Ind. Stated purity, used Further purification Redistilled; no fur given.	S: grade (Wako Ltd.), no d without on. rther details
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta After thermal equilibri lished a recirculating was used to vaporize li to transport the vapor containing (2). Five 1 were withdrawn into sep funnels. The concentra	AUXILIARY r to an and is the paper. 10-20 cm ³ of in separate tted flasks. um was estab- stream of air quid (1) and to the flask 0 cm ³ aliquots aratory tion of (1) in by extraction d by UV-	INFORMAT SOURCE A (1) P I S f (2) F S S S S S S S S S S S S S S S S S S S	TION AND PURITY OF MATERIAL Pure Chemical Ind. Stated purity, used Stated purity, used	S: grade (Wako Ltd.), no d without on. rther details
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta After thermal equilibri lished a recirculating was used to vaporize li to transport the vapor containing (2). Five 1 were withdrawn into sep funnels. The concentra (2) was then determined into chloroform followe spectrophotometry. Sta spectrophotometry were	r to an and is the paper. 10-20 cm ³ of in separate tted flasks. um was estab- stream of air quid (1) and to the flask 0 cm ³ aliquots aratory tion of (1) in by extraction d by UV- ndards for the prepared by	INFORMAT SOURCE A (1) P I S f (2) F S S S S S S S S S S S S S S S S S S S	TION AND PURITY OF MATERIAL Pure Chemical Ind. Stated purity, used Stated purity, used	S: grade (Wako Ltd.), no d without on. rther details
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta After thermal equilibri lished a recirculating was used to vaporize li to transport the vapor containing (2). Five 1 were withdrawn into sep funnels. The concentra (2) was then determined into chloroform followe spectrophotometry. Sta	r to an and is the paper. 10-20 cm ³ of in separate tted flasks. um was estab- stream of air quid (1) and to the flask 0 cm ³ aliquots aratory tion of (1) in by extraction d by UV- ndards for the prepared by	INFORMAT SOURCE A (1) P I Soly F Specif temp. REFEREN	TION AND PURITY OF MATERIAL Pure Chemical Ind. Stated purity, used Stated purity, used	S: grade (Wako Ltd.), no d without on. rther details
the same temperatur METHOD/APPARATUS/PROCEDURE: The apparatus is simila earlier design (ref 2) described in detail in 100-200 cm ³ of (2) and liquid (1) were placed but connected thermosta After thermal equilibri lished a recirculating was used to vaporize li to transport the vapor containing (2). Five 1 were withdrawn into sep funnels. The concentra (2) was then determined into chloroform followe spectrophotometry. Sta spectrophotometry were	r to an and is the paper. 10-20 cm ³ of in separate tted flasks. um was estab- stream of air quid (1) and to the flask 0 cm ³ aliquots aratory tion of (1) in by extraction d by UV- ndards for the prepared by	INFORMAT SOURCE A (1) P I (2) F (2) F (2) F (2) Soly. Specif temp. REFEREN 1. Ke	TION AND PURITY OF MATERIAL Pure Chemical Ind. Stated purity, used Stated purity, used	S: grade (Wako Ltd.), no i without on. rther details f error not

COMPONENTS: (1) Propylbenzene; C₉H₁₂; [103-65-1] (2) Water; H₂O; [7732-18-5] Bull. Chem. Soc. Jpn. <u>1984</u>, 57, 1539-44.

VARIABLES:	PREPARED BY:
One Temperature: 25°C	G.T. Hefter

# EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be  $3.76 \times 10^{-4} \mod(1)/\text{dm}^3 \text{ sln}$ . Assuming a solution density of  $1.00 \text{ kg/dm}^3$  this corresponds to a solubility of  $4.52 \times 10^{-3} \text{ g}(1)/100 \text{ g sln}$ ,  $x_1 = 6.78 \times 10^{-6}$ , calculated by the compiler.

AUXILIARY INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS;	
The apparatus used is described in detail in ref 1. The method involves the introduction of solute vapor(1) into liquid (2) by bubbling air through liquid (1) using a recirculat- ing pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analysed by solvent extraction - UV spectro- photometry.	<ol> <li>Analytical reagent grade source and purity not stated, used without further purification.</li> <li>Deionized and redistilled; no further details given.</li> </ol>	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	
	1. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u> , 55, 1054-62.	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1,8-Nonadiyne; C ₉ H ₁₂ ; [2396-65-8]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and
	A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of 1,8-nonadiyne in wa to be 125 g(1)/10 ⁶ g(2). The corresponding mass percent and ma by the compilers are 0.0125 g(1)/100	ble fraction, $x_1$ , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromato- graphed in conjunction with a flame- ionization detector.	<ul> <li>(1) Phillips Petroleum or Columbia Chemical; used as received.</li> <li>(2) distilled.</li> <li>ESTIMATED ERROR: temp. ± 1.5°C soly. 3 g(1)/10⁶ g(2) (standard deviation of mean)</li> <li>REFERENCES:</li> </ul>

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Nonyne; C ₉ H ₁₆ ; [3452-09-3]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of 1-nonyne in water a	t 25°C was reported
to be 7.2 $g(1)/10^6 g(2)$ .	
The corresponding mass percent and mo	le fraction, $x_1$ , calculated
by the compilers are 0.00072 g(1)/100	g sln and $1.0^{1} \times 10^{-6}$ .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or	(1) Phillips Petroleum or Columbia Chemical; used
magnetically stirred for 1 day,	as received.
with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to	(2) distilled.
allow droplets of undissolved (1) to separate. Absence of emulsion	
was checked microscopically. A	
sample of the hydrocarbon-saturated water was withdrawn with a Hamilton	
syringe and gas liquid chromato-	
graphed in conjunction with a flame- ionization detector.	ESTIMATED ERROR:
	temp. $\pm 1.5^{\circ}C$ soly. 0.5 g(1)/10 ⁶ g(2)
	(standard deviation of mean)
	REFERENCES:
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Components :	ORIGINAL MEASUREMENTS:
<pre>(1) Butylcyclopentane; C₉H₁₈; [2040-95-1]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of Water :	in Butylcyclopentane
<u>t/°C g(2)/100 g slr</u>	$10^4 x_2$ (compiler)
10 0.0056 20 0.0095 30 0.0151	3.93 6.66 10.58
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(1) Not specified.
for 5 hrs. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was	(2) Not specified.
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1,1,3-Trimethylcyclohexane; C₉H₁₈; [3073-66-3] (2) Water; H₂O; [7732-18-5]</pre>	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1,1,3-trimethylcycl and at system pressure was reported to corresponding mass percent and mole for the compiler are 1.77 x 10 ⁻⁴ g(1)/100	to be 1.77 mg(l)/kg(2). The fraction, x ₁ , calculated by
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<ul> <li>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>(2) distilled.</li> <li>ESTIMATED ERROR: temp. ± 1°C soly. ± 0.05 mg(1)/kg(2)</li> </ul>
	SOLY. ± 0.05 mg(1)/kg(2) REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>1,1,3-Trimethylcyclohexane;</li> </ol>	Krzyzanowska, T.; Szeliga, J.
C ₉ H ₁₈ ; [3073-66-3]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

## EXPERIMENTAL VALUES:

The solubility of 1,1,3-trimethylcyclohexane in water at 25°C was reported to be 0.115 mg(l)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 1.15 x  $10^{-5}$  g(1)/100 g sln and 1.64 x  $10^{-8}$ .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

#### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>

	EVALUATOR:
COMPONENTS:	G.T. Hefter, School of Mathematical
(1) 2,2,5-Trimethylhexane; C ₉ H ₂₀ ; [3522-94-9]	and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of
(2) Water; H ₂ O; [7732-18-5]	Chemistry, University of Leuven, Belgium.
	December 1985.

## CRITICAL EVALUATION:

Quantitative solubility data for the 2,2,5-trimethylhexane (1) and water (2) system have been reported in the publications listed in Table 1.

#### TABLE 1: Quantitative Solubility Studies of the 2,2,5-Trimethylhexane (1) - Water (2) System

Reference	T/K	Solubility	Method
McAuliffe (ref 1)	298	(l) in (2)	GLC
Polak and Lu (ref 2)	273,298	mutual	GLC, Karl Fischer

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF 2,2,5-TRIMETHYLHEXANE (1) IN WATER (2)

All the available data on the solubility of 2,2,5-trimethylhexane in water are summarized in Table 2.

At 298K, the only temperature where comparison is possible, the values of McAuliffe (ref 1) and Polak and Lu (ref 2) are in poor agreement (Table 2). The only other value available is that of Polak and Lu at 273K. Thus all solubility values must be regarded as very Tentative in the absence of confirmatory studies.

				Solubility	of
2,2,5-	Trimethylhe	exane (1)	) in Wa	iter (2)	

<i>т/</i> к	Solubili	ty values	
	Reported values 10 ⁴ g(1)/100g sln	"Best" value 10 ⁴ g(1)/100g sln	
273	1.79 (ref 2)	0.8	1.1
298	l.15 (ref 1), 0.54 (ref 2)	0.8 ± 0.3	1.1

a Obtained by averaging where appropriate;  $\sigma_{\rm n}$  has no statistical signigicance.

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(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) 2,2,5-Trimethylhexane; C₉H₂₀; [3522-94-9] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.
	December 1985.

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN 2,2,5-TRIMETHYLHEXANE (1)

Only the data of Polak and Lu (ref 2) are available for the solubility of water in 2,2,5-trimethylhexane and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental values; however, it may be noted that the data of Polak and Lu (ref 2) are generally reliable.

REFERENCES

1. McAuliffe, C. J. Phys. Chem. <u>1966</u>, 70, 1267-75.

2. Polak, J.; Lu, B.C.-Y. Can. J. Chem. 1973, 51, 4018-23.

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 2,2,5-Trimethylhexane; C₉H₂₀; [3522-94-9]</pre>	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
(_,	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	A
The solubility of 2,2,5-trimethylhex. be 1.15 mg (1)/kg sln. The corresponding mole fraction, $x_1$ , is 1.62 x 10 ⁻⁷ . The same value is also reported in r	calculated by the compiler,
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) drop- lets. Absence of emulsion was checked microscopically. A 50 µL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the frac- tionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.	<ul> <li>(1) Phillips Petroleum Co.; 99+% purity; used as received.</li> <li>(2) distilled.</li> <li>ESTIMATED ERROR: temp. ± 1.5°C solv 0 008 mg (1)/kg slp (standard)</li> </ul>

MPONENTS:		ORIGINAL MEASUREMEN	TS:
(1) 2,2,5-Tr: [3522-94	imethylhexane; C ₉ H ₂₀ ; -91	Polak, J.; Lu,	В.С-Ү.
-	-	Can. J. Chem.	<u>1973</u> , <i>51</i> , 4018-23.
(2) water; H.	₂ 0; [7732-18-5]		
ARIABLES:		PREPARED BY:	
Temperature:	0-25°C	M.C. Haulait-P	irson
Temperature.	·		
XPERIMENTAL VALU	ES:		
	Solubility of 2,2,5-tri	methylhexane in v	water
t/°C	mg(1)/kg	sln	$x_1$ (compiler)
		<u>с</u>	$1.11 \times 10^{-7}$
25 ^b	0.79		$7.58 \times 10^{-8}$
45	010-1		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
	Solubility of water in	2,2,5-trimethylh	exane
t/°C	mg(2)/kg	sln	x2 (compiler)
0 ^a	25 ^d		$1.78 \times 10^{-4}$
25 ^b	75 ^d "Estimated Error"		5.34 x 10 ⁻⁴
25 ^b			5.34 x 10 ⁻⁴
25 ^b	"Estimated Error"	INFORMATION	5.34 x 10 ⁻⁴
a-e See	"Estimated Error" AUXILIARY	INFORMATION	
25 ^b a-e See METHOD/APPARATUS	"Estimated Error" AUXILIARY	SOURCE AND PURITY O	DF MATERIALS:
25 ^b a-e See ETHOD/APPARATUS, The solubili determined b	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography.	SOURCE AND PURITY ( (1) Phillips P grade reag	DF MATERIALS; etroleum Co.; pure ent (99%+); shaken
25 ^b a-e See ÆTHOD/APPARATUS, The solubili determined b The solubili	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was	SOURCE AND PURITY ( (1) Phillips P grade reag	OF MATERIALS; etroleum Co.; pure
25 ^b a-e See ETHOD/APPARATUS, The solubili determined b The solubili determined b tion. 50 mL	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with	SOURCE AND PURITY ( (1) Phillips P grade reag three time water.	DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled
25 ^b a-e See ETHOD/APPARATUS, The solubili determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon	SOURCE AND PURITY ( (1) Phillips P grade reag three time	DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled
25 ^b a-e See METHOD/APPARATUS, The solubili determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial coated rubbe a constant-to	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon r septum and placed in emperature water bath.	SOURCE AND PURITY ( (1) Phillips P grade reag three time water.	DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled
25 ^b a-e See METHOD/APPARATUS, The solubili determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial coated rubbe a constant-t. The system w	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon r septum and placed in emperature water bath. as stirred magnetical-	SOURCE AND PURITY ( (1) Phillips P grade reag three time water.	DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled
25 ^b a-e See WETHOD/APPARATUS, The solubili determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial coated rubbe a constant-t The system w ly for 24 hr bath without	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon r septum and placed in emperature water bath. as stirred magnetical- or was kept in the stirring for at least	SOURCE AND PURITY ( (1) Phillips P grade reag three time water.	DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled
25 ^b a-e See WETHOD/APPARATUS. The solubili determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial coated rubbe a constant-t. The system w ly for 24 hr bath without 7 days befor for analysis	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon r septum and placed in emperature water bath. as stirred magnetical- or was kept in the	SOURCE AND PURITY ( (1) Phillips P grade reag three time water. (2) distilled.	<pre>DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled 2°C; b) ± 0.01°C d) ± 4.7%;</pre>
25 ^b a-e See WETHOD/APPARATUS. The solubili determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial coated rubbe a constant-t. The system w ly for 24 hr bath without 7 days befor for analysis	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon r septum and placed in emperature water bath. as stirred magnetical- or was kept in the stirring for at least e samples were taken . Details of the	SOURCE AND PURITY ( (1) Phillips P grade reag three time water. (2) distilled. ESTIMATED ERROR: temp. a) ± 0.0 soly. c) ± 4%;	<pre>DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled 2°C; b) ± 0.01°C d) ± 4.7%;</pre>
25 ^b a-e See WETHOD/APPARATUS. The solubili determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial coated rubbe a constant-t. The system w ly for 24 hr bath without 7 days befor for analysis	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon r septum and placed in emperature water bath. as stirred magnetical- or was kept in the stirring for at least e samples were taken . Details of the	<pre>SOURCE AND PURITY (  (1) Phillips P   grade reag   three time   water.  (2) distilled.  ESTIMATED ERROR:   temp. a) ± 0.0   soly. c) ± 4%;       e) ± 3.1</pre>	<pre>DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled 2°C; b) ± 0.01°C d) ± 4.7%;</pre>
25 ^b a-e See WETHOD/APPARATUS. The solubili determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial coated rubbe a constant-t. The system w ly for 24 hr bath without 7 days befor for analysis	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon r septum and placed in emperature water bath. as stirred magnetical- or was kept in the stirring for at least e samples were taken . Details of the	<pre>SOURCE AND PURITY (  (1) Phillips P   grade reag   three time   water.  (2) distilled.  ESTIMATED ERROR:   temp. a) ± 0.0   soly. c) ± 4%;       e) ± 3.1</pre>	<pre>DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled 2°C; b) ± 0.01°C d) ± 4.7%;</pre>
25 ^b a-e See WETHOD/APPARATUS. The solubili determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial coated rubbe a constant-t. The system w ly for 24 hr bath without 7 days befor for analysis	"Estimated Error" AUXILIARY /PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon r septum and placed in emperature water bath. as stirred magnetical- or was kept in the stirring for at least e samples were taken . Details of the	<pre>SOURCE AND PURITY (  (1) Phillips P   grade reag   three time   water.  (2) distilled.  ESTIMATED ERROR:   temp. a) ± 0.0   soly. c) ± 4%;       e) ± 3.1</pre>	<pre>DF MATERIALS: etroleum Co.; pure ent (99%+); shaken s with distilled 2°C; b) ± 0.01°C d) ± 4.7%;</pre>

OMPONENTS:	ORI	GINAL MEASUREMENTS:
(1) 2,6-Dimethylheptane; C ₉ H [1072-05-5]	20; En	glin, B.A.; Plate, A.F.; Tugolukov V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	] <i>Kh</i>	im. Tekhnol. Topl. Masel <u>1965</u> , 10, 42 <b>-</b> 6.
VARIABLES:	PRE	PARED BY:
Temperature: 10-50°C	A.	Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	──── <b>─</b> ┖ _{───}	
Solubility of	Water in 2,	6-dimethylheptane
<u>t/°C</u> g(2),	/100 g sln	10 ⁴ x ₂ (compiler)
	0.0053 0.0091	3.77 6.48
30	0.0160	11.39
	0.0301 0.0465	21.40 33.02
	AUXILIARY INFO	
Component (1) was introduced	into a (	RCE AND PURITY OF MATERIALS:
Component (1) was introduced thermostatted flask and satur for 5 hours with (2). Next,	into a ( rated calcium (	
Component (1) was introduced thermostatted flask and satur for 5 hours with (2). Next, hydride was added and the evo hydrogen volume measured and the concentration of (2) in	into a ( rated calcium ( plving hence	RCE AND PURITY OF MATERIALS: 1) Not specified.
Component (1) was introduced thermostatted flask and satur for 5 hours with (2). Next, hydride was added and the evo hydrogen volume measured and the concentration of (2) in	into a ( rated calcium ( olving hence (1) was	RCE AND PURITY OF MATERIALS: 1) Not specified. 2) Not specified.
Component (1) was introduced thermostatted flask and satur for 5 hours with (2). Next, hydride was added and the evo hydrogen volume measured and the concentration of (2) in	into a ( rated calcium ( olving hence (1) was	RCE AND PURITY OF MATERIALS: 1) Not specified. 2) Not specified. TIMATED ERROR:
Component (1) was introduced thermostatted flask and satur for 5 hours with (2). Next, hydride was added and the evo hydrogen volume measured and the concentration of (2) in	into a ( rated calcium ( olving hence (1) was	RCE AND PURITY OF MATERIALS: 1) Not specified. 2) Not specified.
Component (1) was introduced thermostatted flask and satur for 5 hours with (2). Next, hydride was added and the evo hydrogen volume measured and the concentration of (2) in	into a ( rated calcium ( olving hence (1) was ES'	RCE AND PURITY OF MATERIALS: 1) Not specified. 2) Not specified. TIMATED ERROR:
Component (1) was introduced thermostatted flask and satur for 5 hours with (2). Next, hydride was added and the evo hydrogen volume measured and the concentration of (2) in	into a ( rated calcium ( olving hence (1) was ES'	RCE AND PURITY OF MATERIALS: 1) Not specified. 2) Not specified. TIMATED ERROR: bt specified.
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced thermostatted flask and satur for 5 hours with (2). Next, hydride was added and the evo hydrogen volume measured and the concentration of (2) in evaluated.	into a ( rated calcium ( olving hence (1) was ES'	RCE AND PURITY OF MATERIALS: 1) Not specified. 2) Not specified. TIMATED ERROR: bt specified.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2-Methyloctane; C ₉ H ₂₀ ; [3221-61-2]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of Water	in 2-methyloctane
<u>t/°C</u> <u>g(2)/100 g sln</u>	$10^4 x_2$ (compiler)
10 0.0052 20 0.0090 30 0.0156	3.70 6.41 11.10
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hours with (2). Next, calcium	(1) Not specified.
hydride was added and the evolving hydrogen volume measured and hence	
the concentration of (2) in (1) was evaluated.	
-raiuateu.	
	ESTIMATED ERROR:
1	
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methyloctane; C ₉ H ₂₀ ; [2216-33-3]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of Water	in 3-methyloctane
<u>t/°C</u> <u>g(2)/100 g s</u> ]	$\frac{10^4 x_2}{(\text{compiler})}$
10         0.0050           20         0.0087           30         0.0155	3.56 6.20 11.03
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(l) Not specified.
for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 4-Methyloctane; C ₉ H ₂₀ ;	Price, L.C.
[2216-34-4] (2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
(2) water, m ₂ o, [,,52 10 5]	,,
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 4-methyloctane in pressure was reported to be 0.115 mg mass percent and mole fraction, $x_1$ , are 1.15 x 10 ⁻⁵ g(1)/100 g sln and 1	<pre>(1)/kg(2). The corresponding calculated by the compiler</pre>
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<ol> <li>Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>distilled.</li> </ol>
	ESTIMATED ERROR:
	<pre>temp. ± 1°C soly. ± 0.011 mg(1)/kg(2)</pre>
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 4-Methyloctane; C₉H₂₀;</pre>	Krzyzanowska, T.; Szeliga, J.
[2216-34-4]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 4-methyloctane to be 0.115 mg(l)/kg(2).	e in water at 25°C was reported
The corresponding mass percent a	and mole fraction, $x_1$ , calculated
by compiler are 1.15 x $10^{-5}$ g(1)	

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

## AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The saturated solutions of (1) in (1) not specified. (2) were prepared in two ways. First, 200  $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) (2) not specified. and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh ESTIMATED ERROR: Porasil column (70°C) and a flame ionization detector was used. Sat-urated solutions of heptane in (2) soly. 0.02 mg(1)/kg(2) (standard were used as standard solutions. deviation from 7-9 determinations). **REFERENCES:** 

COMPONENTS:	EVALUATOR:
<pre>(1) Nonane; C₉H₂₀; [111-84-2] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	February 1986.

CRITICAL EVALUATION: (continued)

TABLE	2.	Tent	ativ	ze s	Solubi	lity	Values	for
	Not	nane	(1)	in	Water	(2)		

T/K	Solubili	Solubility values			
	Reported values ^a	"Best" val	ues $(\pm \sigma_n)^b$ $10^8 x_1$		
	10 ⁵ g(1)/100g sln	10 ⁵ g(1)/100g sln	10 ⁸ ″ _x 1		
293	2.89 (ref 8)	2.9	4.1		
298	2.2 (ref 2), 0.71 (ref 5), 1.22 (ref 6), 2.72 (ref 8)	1.7 ± 0.8	2.4		
303	1.4* (ref 6)	1.4	2.0		
313	1.7* (ref 6)	1.7	2.4		
323	2.2* (ref 6)	2.2	3.1		
333	2.6* (ref 6)	2.6	3.7		
343	3.1* (ref 6)	3.1	4.4		
353	3.4* (ref 6)	3.4	4.8		
363	3.7* (ref 6)	3.7	5.2		
373	4.2* (ref 6)	4.2	5.9		
383	8.0* (ref 6)	8.0	11		
393	16* (ref 6)	16	22		
403	32* (ref 6)	32	45		

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the author's original data. b Obtained by averaging where appropriate;  $\sigma_n$  has no statistical signifi-

# 2. SOLUBILITY OF WATER (2) IN NONANE (1)

Only the single point data of Schatzberg (ref 1) at 298K and Benkovski et al. (ref 3) at 303K are available for the solubility of water in nonane and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheets for the experimental values; however, it may be noted that the data of Schatzberg (ref 1) are generally reliable.

## REFERENCES

cance.

- 1. Schatzberg, P. J. Phys. Chem. <u>1963</u>, 67, 776-9.
- 2. McAuliffe, C. Science 1969, 163, 478-9.
- Benkovski, V.G.; Nauruzov, M.H.; Bogoslovskaya, T.M. Tr. Inst. Khim. Nefti Prir. Solei Alkad. Nauk Kaz. SSR <u>1970</u>, 2, 25-32.
- 4. Roof, J.G. J. Chem. Eng. Data <u>1970</u>, 15, 301-3.
- 5. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u>, 13, 885-7.

(continued next page)

COMPONENTS:	EVALUATOR:
(2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the nonane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1. Quantitative Solubility Studies ofthe Nonane (1) - Water (2) System			
Reference	T/K	Solubility	Method
Schatzberg (ref 1)	298	(2) in (1)	Karl Fischer
McAuliffe (ref 2)	298	(1) in (2)	GLC
Benkovski <i>et al</i> . (ref 3)	303	(2) in (1)	Karl Fischer
Krasnoshchekova and Gubergrits (ref 5)	298	(1) in (2)	GLC
Price (ref 6)	298-410	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 7)	298	(1) in (2)	GLC
Jonsson et al. (ref 8)	288,293	(1) in (2)	partition coeff.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Roof (ref 4) has also reported a three phase critical point of unspecified composition at 555K and 8.5 MPa. For convenience further discussion of this system will be in two parts.

# 1. SOLUBILITY OF NONANE (1) IN WATER (2)

All the data available for the solubility of nonane in water are summarized in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 7) which does not appear to be independent of that of Price (ref 6) and has therefore been excluded from consideration.

At 298K, the only temperature where comparison is possible, the agreement between the various studies is poor (Table 2) and the average must be regarded as Tentative only. Interestingly, the average value of  $1.7 \times 10^{-5}$  g(1)/100g sln is, however, quite close to the value of  $2.0 \times 10^{-5}$  g(1)g sln predicted by extrapolation of the lower *n*-alkane solubilities.

At other temperatures only the data of Jonsson  $et \ al$ . (ref 8) at 293K and Price (ref 6) at 303-410K are available and thus no Critical Evaluation is possible. There are also insufficient independent data to warrant plotting.

COMPONENTS:	EVALUATOR:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

- 6. Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u>, 60, 213-44.
- 7. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.
- Jonsson, J.A.; Vejrosta, J.; Novak, J. Fluid Phase Equil. <u>1982</u>, 9, 279-86.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	Schatzberg, P.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
EAFERIMENTAL VALUES.	
The solubility of water in nonane at	25°C was reported to be
79 mg(2)/kg sln corresponding to a mo	
	2
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was saturated by storing over a layer of (2) in a brown glass bottle	(1) Phillips Petroleum Co.; research grade; 99.69 mole%; passed
without any agitation. The bottle	repeatedly through a column
was sealed with serum cap and com- pletely submerged in the water-bath	of silica gel until no absorp- tion occurred in the 220 to
for 7 days. A 20-mL sample was withdrawn with a silicone-hydro-	340 nm spectral range.
phobized hypodermic syringe. Sta-	(2) distilled and deionized.
bilized Karl Fischer reagent diluted to a titer of $1.0-1.3 \text{ mg}(2)/\text{mL}$ was	
used to titrate (2) in (1) directly in the presence of methanol to a	ESTIMATED ERROR:
"dead-stop" end-point using a Beckman KF3 automatic titrimeter.	temp. ± 0.02°C soly. 0-6% (deviations from the mean)
beckman KFS automatic titrimeter.	sory. 0-6% (deviations from the mean)
	REFERENCES:
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Science <u>1969</u> , 163, 478 <b>-</b> 9.
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of nonane in water at 0.220 mg(l)/kg(2). The corresponding mass percent and moby the compiler are 2.2 x 10 ⁻⁵ g(l)/l	ble fraction, $x_1$ , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaker for 2 minutes. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.	(2) distilled.
	ESTIMATED ERROR:
	soly. ± 0.021 mg(1)/kg(2)
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2] (2) Water; H ₂ O; [7732-18-5]	Benkovski, V.G.; Nauruzov, M.H.; Bogoslovskaya, T.M. Tr. Inst. Khim. Nefti Prir. Solei Akad. Nauk Kaz. SSR <u>1970</u> , 2, 25-32.
VARIABLES:	PREPARED BY:
One temperature: 303 K	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of water in nonane at 0.0045 g(2)/100 g sln. The corresponding mole fraction, $x_2$ , is 0.00032.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Equal volumes of (1) and (2) were placed in a glass cylinder and periodically shaken for 6 h, then sampled and analyzed by the Karl Fischer method.	<pre>SOURCE AND PURITY OF MATERIALS: (1) source not specified; purified; purity not specified. (2) distilled. ESTIMATED ERROR:</pre>
	ESTIMATED ERROR: Not specified
	REFERENCES :

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya.
(2) Water; H ₂ O; [7732-18-5]	-
2	Neftekhimiya <u>1973</u> , 13, 885-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of nonane in water at	25°C was reported to be
$x_1 = 1.00 \times 10^{-8}$ .	
The corresponding mass percent calcul	ated by the compiler is
7.1 x $10^{-6}$ g(1)/100 g sln.	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 10 mL (1) and 300 mL	(1) source not specified;
(2) was placed in a double-walled bottom-stoppered vessel and vigor-	CP reagent; purity not specified.
ously stirred magnetically for 10-	(2) distilled.
12 hr. The phases were allowed to separate; a first sample of the	
water phase was rejected and next 200 mL of this phase was taken,	
20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was	
allowed to equilibrate with the air,	ESTIMATED ERROR:
and the (1)-saturated air was analyzed by glc.	
	not specified.
	REFERENCES :
	ALL DREIVED ;
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(1) Nonane; C ₉ H ₂₀ ; [111-84-2] (2) Water; H ₂ O; [7732-18-5]		Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.		
VARIABLES:		PREPARED BY:		
Temperature: 25-	136.6°C	F. Kapuku		
EXPERIMENTAL VALUES:	<u></u>			
Solub	ility of nonane in wa	ter at system pressur	e	
t/°C	mg(1)/kg(2)	g(l)/100 g sln (compiler)	10 ⁸ x1 (compiler)	
25.0	0.122 ± 0.007	0.0000122	1.71	
69.7	0.309 ± 0.019	0.0000309	4.34	
99.1	$0.420 \pm 0.034$	0.0000420	5.90	
121.3	1.70 ± 0.11	0.000170	23.9	
136.6	5.07 ± 0.25	0.000507	71.2	
	AUXILIARY	INFORMATION		
METHOD/APPARATUS/PRO		SOURCE AND PURITY OF MATE	RTALS:	
Room-temperature determined by us tubes. The (1) of (2) and insur to 4 days) of th High-temperature carried out in t chromatograph. contained in 75 stainless steel Modified Micro I the bottom of th lowed syringe ac during sampling.	e solubilities were se of screw-cap test phase floated on top red saturation (in 2 he aqueous phase. solubility work was the ovens of the gas The solutions were mL double ended sample cylinders. inear Valves sealed he cylinder and al- ccess to the solution The sample is then	<ul> <li>(1) Phillips Petrole 99+%.</li> <li>(2) distilled.</li> </ul> ESTIMATED ERROR: temp. ± 1°C solv. range of value.	aum Company;	
during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.			es given above	

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ORIGINAL MEASUREMENTS:

232 COMPONENTS:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	Krzyzanowska, T.; Szeliga, J.		
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	M.C. Haulait-Pirson		

#### EXPERIMENTAL VALUES:

The solubility of nonane in water at 25°C was reported to be 0.122 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 1.22 x  $10^{-5}$  g(1)/100 g sln and 1.71 x  $10^{-8}$ .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

(1) Nonane; C₉H₂₀; [111-84-2] Jonsson, J.A.; Vejrosta, J.; Novak, J. (2) Water; H₂O; [7732-18-5] Fluid Phase Equil. 1982, 9, 279-86. VARIABLES: PREPARED BY: Temperature: 15-20°C G.T. Hefter EXPERIMENTAL VALUES: Solubility of nonane (1) in water (2) t∕°C  $10^{8} \times 1$ 10⁵g(l)/100g sln mg(l)/kg sln (compiler) (compiler) 0.289 15 2.89 4.05 20 0.272 2.72 3.81 Solubility values were calculated by the authors from their smoothed air-water partition coefficient ( $K_{\rm AW}$ ) by assuming  $K_{\rm AW}$  values obtained at infinite dilution were valid at the saturation pressure of (1). AUXILIARY INFORMATION METHOD / APPARATUS / PROCEDURE : SOURCE AND PURITY OF MATERIALS: Air-water partition coefficients Fluka, > 99%, used as received. were measured by saturating a portion of water by a stream of (2) Not specified. nitrogen containing a known vapor concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and the entrapped (1) analyzed by gas chromatography. The method and apparatus are described in detail in ref 1. ESTIMATED ERROR: Not specified. **REFERENCES:** Vejrosta, J.; Novak, J.; Jonsson, J.A. Fluid Phase Equil. <u>1982</u>, 8, 25-35. 1.

ORIGINAL MEASUREMENTS:

COMPONENTS :

Particular and the second s	
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.
(2) Seawater	Neftekhimiya <u>1973</u> , 13, 885 <b>-</b> 8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 6 g/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of nonane in seawater	was reported to be
$4.3 \times 10^{-5}$ g(l)/100 g sln. and the co	orresponding mole fraction,
$x_1 = 6.0 \times 10^{-8}$ .	
1 - 0.0 X 10 .	
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution was prepared	(1) "chemically pure"
by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs.	(2) distilled water plus salt
in a flask placed in a temperature	mixture.
controlled bath. A sample of solu- tion was then transferred to a	
closed flask with head space volume	
equal to solution volume. Hydro- carbon concentration in the head	
space was determined by gas chroma-	
tography and the corresponding solution concentration calculated.	ESTIMATED ERROR:
	not specified.
	REFERENCES :
1	

COMPONENTS:	EVALUATOR:
(2) Water: H_O: [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

## CRITICAL EVALUATION:

Quantitative data for the solubility of naphthalene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1	: Quantitative	Studies of	the	Solubility
of	Naphthalene (]	) in Water	(2)	

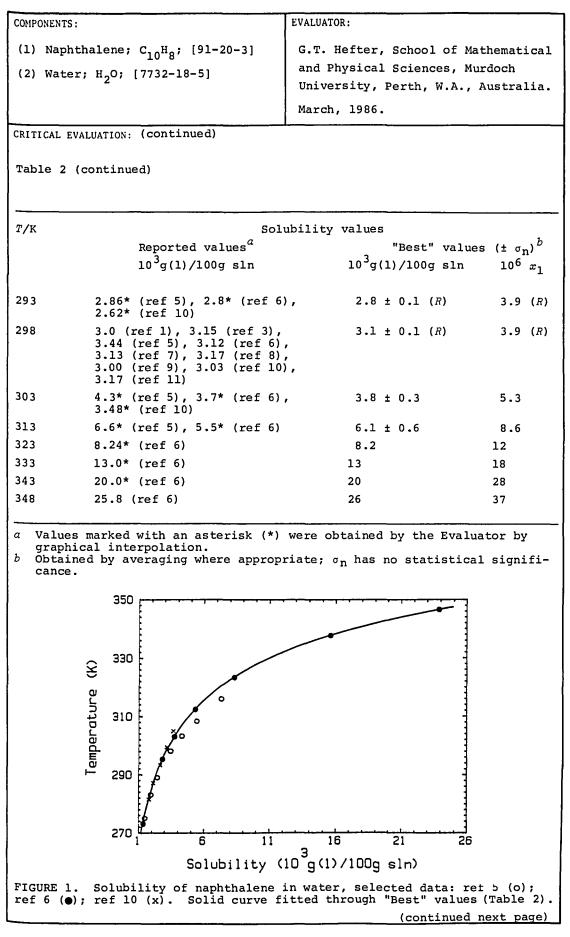
Reference	Т/К	Method
Hilpert (ref 1)	273,298	gravimetric
Mitchell (ref 2)	288,298	interferometric
Andrews and Keefer (ref 3)	298	spectrophotometric
Klevens (ref 4)	298	spectrophotometric
Bohon and Claussen (ref 5)	273-316	spectrophotometric
Wauchope and Getzen (ref 6)	273-348	spectrophotometric
Eganhouse and Calder (ref 7)	298	GLC
Mackay and Shiu (ref 8)	298	spectrofluorometric
Schwarz and Wasik (ref 9)	285-298	spectrophotometric
Schwarz (ref 10)	282-305	spectrophotometric
May et al. (ref 11)	298	HPLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data appear to have been published on the solubility of water in naphthalene.

Despite the low solubility of naphthalene in water the published data are in excellent agreement. With the exception of the 298K data of Mitchell (ref 2) and Klevens (ref 4) which differ markedly from other studies, all the available data are summarized in Table 2. Selected data are also plotted in Figure 1.

TABLE 2:	Recommended (R)				of	the Solubility
	of Naphtha	lene	(1) in Wat	ter (2)		

T/K	Solubili	ty values	_
	Reported values ^a	"Best" values	
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln	10 ⁶ x1
273	1.9 (ref 1), 1.37 (ref 5), 1.37 (ref 6)	1.5 ± 0.2	2.1
283	1.94 (ref 5), 2.0* (ref 6), 1.87* (ref 10)	1.9 ± 0.1 (R)	2.7 (R)
		(Table 2 continued m	ext page)



EVALUATOR: COMPONENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. March, 1986. CRITICAL EVALUATION: (continued) REFERENCES 1. Hilpert, S. Angew. Chem. 1916, 29, 57-9. Mitchell, S. J. Chem. Soc. <u>1926</u>, 129, 1333-6. 2. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1949, 71, 3644-77. 3. 4. Klevens, H.B. J. Phys. Chem. 1950, 54, 283. 5. Bohon, R.L.; Claussen, W.F. J. Am. Chem. Soc. 1951, 73, 1571-8. 6. Wauchope, R.D.; Getzen, F.W.J. Chem. Eng. Data 1972, 17, 38-41. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40, 7. 555-61. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402. 8. 9. Schwarz, F.P.; Wasik, S.P. J. Chem. Eng. Data 1977, 22, 270-3. 10. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7. 11. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. 1978, 50, 997-1000. ACKNOWLEDGEMENT The Evaluator thanks Dr Brian Clare for the graphics.

OMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Hilpert, S.
(2) Water; H ₂ O; [7732-18-5]	Angew. Chem. <u>1916</u> , 29, 57-9.
-	
ARIABLES:	PREPARED BY:
Temperature: 0 and 25°C	A. Maczynski and A. Szafranski
XPERIMENTAL VALUES:	L <u></u>
Solubility of napht	halene in water
$\frac{t/^{\circ}C}{10^3}$	$g(1)/100 g sln = \frac{10^6 x_1}{10^6 x_1}$
0	1.9 2.7
25	3.0 4.2
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A sample of (1) was shaken with $1000 g(2)$ until saturation and then	(1) not specified.
filtered. The filtrate was steam distilled to drive away (1) which was collected and presumably weighed	(2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

NENTS :			

COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Mitchell, S.		
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Soc. London <u>1926</u> , 1332-6.		
2			
VARIABLES:	PREPARED BY:		
Temperature: 15 and 25°C	A. Maczynski and Z. Maczynska		
	l		
EXPERIMENTAL VALUES:			
Solubility of naph	thalene in water		
$t/^{\circ}C$ g(1) L ⁻¹ (2) g(1)/	100 g sln (compiler) $10^{6}x_{1}$ (compiler)		
	0022 3.1 0040 5.6		
25 0.040 0.	5.0		
AUXTLTARY	INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
For this study an interferometer of the type described in ref (1) was	(1) not specified.		
constructed.	(2) not specified.		
]	ESTIMATED ERROR:		
	not specified.		
	not specified.		
	DECEDENCIC.		
	REFERENCES: 1. Jamin Ann. Chim. Phys. <u>1958</u> ,		
	52, 171.		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of naphthalene in wate 0.00315 g(1)/100 g sln. The corresponding mole fraction, $x_1$ , is 4.42 x 10 ⁻⁶ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a mea- sured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorb- ance of the hexane phase was mea- sured against a hexane blank on the	<ol> <li>Eastman Kodak Co., best grade; recrystallized from ethanol; mp. 80.5°C.</li> <li>not specified.</li> </ol>
Beckman spectrophotometer.	ESTIMATED ERROR:
	not specified.
	REFERENCES :

242			
COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Klevens, H.B.		
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.		
VARIABLES:			
	PREPARED BY: M.C. Haulait-Pirson		
Temperature: 25°C	M.C. Haulalt-Pirson		
EXPERIMENTAL VALUES:			
	a at 25% und reported to be		
The solubility of naphthalene in wate 0.0125 g(1) $L^{-1}$ sln and 9.75 x $10^{-5}$	r at 25 C was reported to be mol(1) $L^{-1}$ sln. Assuming that		
1.00 L sln = 1.00 kg sln, the corresp			
compiler are 0.00125 g(1)/100 g sln a			
	-		
	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The solubility of (1) in (2) was determined by shaking small amounts	(1) not specified.		
of (1) in 1 liter of (2) for as long as three months. Aliquots were	(2) not specified.		
removed and concentrations deter- mined by spectra.			
	ESTIMATED ERROR:		
	not specified.		

REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Bohon, R.L.; Claussen, W.F.			
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1951</u> , 73, 1571-8.			
VARIABLES:	PREPARED BY:			
Temperature: 0-42.8°C	G.T. Hefter			
EXPERIMENTAL VALUES:				
$t/^{\circ}C$ 10 ³ g(1).	phthalene in water /100g sln ^a 10 ⁶ x ₁ piler)			
Image: Completify           0.0         1.37         1.92           0.4         1.37         1.92           0.5         1.38         1.94           0.9         1.46         2.05           1.9         1.50         2.11           9.4         1.96         2.75           10.0         1.94         2.72           14.9         2.34         3.29           15.9         2.46         3.45           19.3         2.80,         3.93,           25.0         3.44b         4.83b           25.6         3.58         5.03           30.1         4.30         6.16           35.2         5.45         7.65           36.0         5.48         7.69           42.8         7.35         10.3           a         Solubilities of (1) in (2) were reported as "optical density" (absorbance)           measurements.         Solubilities were calculated by the compiler using the           Beer-Lambert law, the stated cell path-length (1 cm) and the authors'           "extinction coefficients" (absorptivities) and corrected optical           densities.         This gave a solubility of g(1)/L sln which was then           converted to g(1)/100g sln by assumi				
^D Given in the paper as 0.0344g(1)/L s. AUXILIARY	INFORMATION			
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:			
A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.	<ol> <li>Allied Chemical &amp; Dye Corp., purified by vacuum distillation.</li> <li>Air-free conductivity water, no other details given.</li> </ol>			

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Wauchope, R.D.; Getzen, F.W.		
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.		
VARIABLES:	PREPARED BY:		
Temperature: 0-75°C	A. Maczynski		
EXPERIMENTAL VALUES:			
Solubility of napht	halene in water		
mg(1)/kg(2)			
t/°C smoothed wi	$\begin{array}{ccc} th & g(1)/100 \ g \ sln & 10^6 x_1 \\ & (compiler) & (compiler) \end{array}$		
experiment(std dev)			
0.0 13.7(0. 22.2 28.8, 29.1, 28.8 28.3	0 00000 2 00 1		
24 5 30 8(2) 30 1(2) 30 7 30.7	0.00307 4.31		
	2/ 0.00512 1.00		
29.9 38.1, 38.2, 38.3 37.3	0.00373 5.24		
30.3         38.1, 37.6, 37.6         37.8           34.5         44.6, 43.8         44.3	0.00378 5.31 0.00443 6.23		
34.5       44.6, 43.8       44.3         39.2       52.6, 52.8       53.3         40.1       54.8       55.0	0.00533 7.49		
40.1 54.8 55.0	0.00550 7.73		
40.1         54.8         55.0           44.7         66.0, 65.5, 65.3         66.2           50.0         82.4 (0.	0.00662         9.30           4)         0.00824         11.58		
50.0 82.4(0. 50.2 78.6 83.1	4) 0.00824 11.58 0.00831 11.68		
55.6 106 105	0.0105 14.8		
64.5 166, 151, 157 156	0.0156 21.9		
73.4     240, 247, 244     239       75.0     258(3)	0.0239 33.6 0.0258 36.3		
AUXILIARY	INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS;		
Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer	<ol> <li>Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.</li> <li>distilled and deionized.</li> </ol>		
after extraction indicated complete			
extraction. Standard solutions were prepared	ESTIMATED ERROR:		
either by direct weighing using a	temp. ± 0.5°C		
Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by	soly. see experimental values above		
serial dilution in calibrated glass-			
ware.	REFERENCES :		
L			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Eganhouse, R.P.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of naphthalene in wate be 31.3 mg(1)/kg(2) and 2.43 x $10^{-4}$ m	
The corresponding mass percent and moby the compiler are $3.13 \times 10^{-3} g(1)/$	the fraction, $x_1$ , calculated 100 g sln and 4.40 x $10^{-6}$ .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating	analytical grade; used as received; no impurities by
columns and flame ionization detec- tors was employed.	
	ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.4 mg(1)/kg(2) (from eight determinations)
	REFERENCES :

.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Mackay, D.; Shiu, W.Y.		
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
The solubility of naphthalene in wat to be 31.7 mg(l) $dm^{-3}$ sln and $x_1 = 4$	$.46 \times 10^{-6}$ .		
The corresponding mass percent calcu is 0.00317 g(l)/100 g sln.	lated by the compiler		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman	<ol> <li>Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.</li> <li>doubly distilled.</li> </ol>		
spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. $\pm$ 0.26 mg(l) dm ⁻³ sln (maximum deviation from several determina- tions).		
	REFERENCES:		

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COMPONENTS:		ORIGINAL MEASUREMENTS:		
		ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Schwarz, F.P.		
(2) Water; H ₂ O; [7732-18-5]		J. Chem. Eng. Data <u>1977</u> , 22, 273-7.		
-				
VARIABLES:		PREPARED BY:		
Temperature: 8.4-	-31.8°C	A. Maczynski		
EXPERIMENTAL VALUES:				
	Solubility of napht	halene in water		
t/°C	$10^4 \text{ mol}(1) \text{ L}^{-1}$			
		(compiler)	(compiler)	
8.4	1.40 ± 0.02	1.79	2.52	
11.1	1.49 ± 0.03	1.91	2.68	
14.0	1.66 ± 0.05	2.13	2.99	
17.5	1.88 ± 0.03	2.41	3.39	
20.2	2.07 ± 0.02	2.65	3.73	
23.2	2.22 ± 0.03	2.85	4.00	
25.0	2.36 ± 0.02	3.03	4.25	
26.3	$2.48 \pm 0.02$	3.18	4.47	
29.2	2.68 ± 0.02	3.44	4.83	
31.8	2.83 ± 0.02	3.63	5.10	
	AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROC	·····	SOURCE AND PURITY OF MATERIALS:		
		[		
Two methods were	used.	(1) source not specifi than 99.9 mole%, b		
At 25°C the solub was determined fr	ility of (1) in (2)	used as received.		
measurements and standard at other At other temperat	was used as a temperatures.	(2) distilled over KMn and passed through column.		
The sealed fluore	scence cells			
contained 5 mL of	the aqueous excess of (1) were			
rotated at least	72 h in a water	ESTIMATED ERROR:		
bath, then remove dry and placed in	d, quickly wiped the fluorimeter.	temp. ± 0.1°C soly. see above		
		REFERENCES:		

COMPONENTS :	ORIGINAL MEASUREMENTS:		
CONFORMIS:	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Schwarz, F.P.; Wasik, S.P.		
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 270-3.		
VARIABLES:	PREPARED BY:		
Temperature: 12-25°C	A. Maczynski		
EXPERIMENTAL VALUES:			
Solubility of napht			
$t/^{\circ}C$ 10 ⁴ mol(1) L ⁻¹	$\begin{array}{ccc} 10^{3} \text{ g(l)/100 g sln} & 10^{6} x_{1} \\ \underline{\qquad (compiler)} & (compiler) \end{array}$		
12 1.57	2.01 2.83		
18 1.90	2.43 3.42		
25 2.34	3.00 4.21		
AUXILIARY	INFORMATION		
METHOD /AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) are too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.	<ol> <li>Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%.</li> <li>distilled from KMnO₄ and passed through a Sephadex column.</li> </ol>		
	ESTIMATED ERROR:		
	temp. $\pm 0.1^{\circ}C$ soly. $\pm 2 \times 10^{-6}$ mol(1) dm ⁻³		
	REFERENCES:		

L

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	May, W.E.; Wasik, S.P.; Freeman, D.H.
(2) Water; H ₂ O; [7732-18-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of naphthalene in wate 31.69 mg(1)/kg(2). The corresponding mass percent and mo by compiler are 0.003169 g(1)/100 g s	ble fraction, $x_1$ , values calculated
	INFORMATION
METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the coupled column liquid chromato- graphic process that has been de- scribed in ref 1.	<pre>SOURCE AND PURITY OF MATERIALS: (1) commercial product; less than 3% impurities. (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). ESTIMATED ERROR: temp. ± 0.05°C soly. ± 0.23 mg(1)/100 kg(2) (standard deviation) REFERENCES: 1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci. <u>1975</u>, 13, 535.</pre>

**EVALUATOR:** COMPONENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA (2) Seawater December 1982 CRITICAL EVALUATION: The solubility of naphthalene (1) in seawater (2) has been reported in six works: Salinity g salts/kg sln  $10^3$  g(1)/100 g sln Authors Method T/K Paul (ref 1) uv spectral 298 30.59 2.53 Gordon and Thorne 2.36 (ref 2)uv spectral 298 35.0 Gordon and Thorne 2.47 (ref 3) 298 31.7 uv spectral Eganhouse and Calder 298 35 2.20 (ref 4) GLC

298

298

30

35.0

At 298 K and a salinity of 35 g salts/kg sln the data of Gordon and Thorne (ref 2), Eganhouse and Calder, and May *et al.* are in good agreement. Therefore the mean value,  $2.29 \times 10^{-3}$ , is adopted as the recommended value at this temperature and salinity. Since the value of Schwarz is lower than would be expected with decreasing salinity, it is considered doubtful. At 298 K and a salinity of 31 g salts/kg sln the data of Paul and of Gordon and Thorne (ref 3) are in fair agreement. Therefore their mean is adopted as a tentative value. Gordon and Thorne (ref 2) and May *et al.* report data for a range of salinities using the Setschenow equation. Schwarz reports data over the temperature range 281 to 303 K. However, since this data at 298 K appears low, the usefulness of this work is diminished.

2.17

2.29

#### REFERENCES

Schwarz (ref 5)

May et al. (ref 6)

1. Paul, M.A. J. Amer. Chem. Soc. 1952, 74, 5274-7.

uv spectral

HPLC

- 2. Gordon, J.E.; Thorne, R.L. J. Phys. Chem. 1967, 71, 4390-9.
- Gordon, J.E.; Thorne, R.L. Geochim. Cosmochim. Acta <u>1967</u>, 31, 2433-43.
   Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.
- 5. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.
- 6. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. 1978, 50, 997-1000.

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ol> <li>Naphthalene; C₁₀H₈; [91-20-3]</li> <li>Sodium chloride; NaC1; [7732-14-5]</li> <li>Water; H₂O; [7647-18-5]</li> </ol>	Paul, M.A. J. Am. Chem. Soc. <u>1952</u> , 74, 5274-7.	
Z VARIABLES:	PREPARED BY:	
One temperature: 25°C		
Salinity: 13-64 g(3)/kg sln	M. Kleinschmidt and W. Shiu	
EXPERIMENTAL VALUES:		
Solubility of Naphthalene	in Aqueous Sodium Chloride	
$g-mol(3)/L^{-1}$ g(2)/kg sln [*] 10 ⁴ g-m	$01(1)/L^{-1}$ 10 ³ Mass & 10 ⁶ x ₁ *	
0.535 30.59 2. 0.771 43.70 1.	37       3.01       4.27         00       2.52       3.61         02       2.53       3.64         68       2.09       3.02         38       1.69       2.48	
AUXILIARY	INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
Equilibration flask: 50-mL glass-	(1) recrystallized from menthanol	
stoppered flask. The flask was heated in a hot-water bath until the hydrocarbon was melted, then shaken	(2) reagent grade, dried at 120°C before weighing	
vigorously while cooling until ex- Cess hydrocarbon had recrystallized.	(3) redistilled	
The flask was then placed into a water bath thermostatically con- trolled at 25.00 ± 0.05°C for at	Sources not specified.	
least 48 hr, and shaken occasionally during that time. Samples were with-		
drawn with a 10-ml transfer pipet, diluted appropriately and analyzed	ESTIMATED ERROR:	
using a spectrophotometer in the ultra-violet region of the spectrum.	temp. ± 0.05°C	
	soly. ± 1 %	
	<b>REFERENCES:</b> 1. Weast, R.C.; CRC Handbook of	
	Chemistry and Physics, 59th Edition; CRC Press <u>1978</u> , pp D299-D300.	
	<i>Chemistry and Physics</i> , 59th Edition; CRC Press 1 <u>978</u> , pp	

COMPONENTS :	ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Gordon, J.E.; Thorne, R.L.			
(2) Sodium chloride; NaCl; [7647-14-5]	J. Phys. Chem. <u>1967</u> , 71, 4390-9.			
(3) Water; H ₂ O; [7732-18-5]				
VARIABLES:	PREPARED BY:			
One temperature: 24.91°C Salinity: 0-108.g(2)/kg.sln EXPERIMENTAL VALUES:	M. Kleinschmidt and D. Shaw			
The solubility of naphthalene in aqueous sodium chloride is reported in terms of the Setschenow equation: $\log(S_0/S) = K_S C_S$ where, S_0 is the solubility of naphthalene in water (mol/L) S is the solubility of naphthalene in solution (mol/L) K_S is the Setschenow constant (L/mol) C_S is the concentration of sodium chloride (mol/L) evaluating the equation for S over the range of C_S 0-2 mol/L, log S_0 = -3.590 ± 0.004 (95% confidence limit) and K_S = 0.220 ± 0.0041 (95% confidence limit). The corresponding mass percent and mole fraction, $x_1$ at salinity = 35 g(2)/kg sln calculated by the compilers are 2.36 x 10 ⁻³ g(1)/100 g sln and 3.48 x 10 ⁻⁶ assuming a solution density of 1.025 kg/L.				
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND FURITY OF MATERIALS:			
Saturated solutions were prepared by equilibrating excess (1) in salt water in sealed ampols for 24 hrs. After filtration the absorbance was measured with a UV spectrophotometer at three wavelengths.	<ul> <li>(1) recrystallized four times and sublimed or zone refined, 99.99+% pure,</li> <li>(2) analytical reagent grade,</li> <li>(3) distilled from potassium per- manganate and redistilled from all glass still.</li> <li>ESTIMATED ERROR:</li> <li>temp. ± 0.03°C soly. see above</li> <li>REFERENCES:</li> </ul>			

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COMPONENTS:	MPONENTS :			ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]		Gordon, J.E.; Thorne, R.L.				
	(2) natural seawater			Geochim. Cosmochim. Acta, <u>1967</u> , 31, 2433-43.		
VARIABLES:		<u></u>		PREPARED BY:		
One tempe	erature: 2	5°C		W.Y. Shiu and	D. Mackay	
Salinity:	10-32 g/	kg sln				
EXPERIMENTA	L VALUES:			~~~~		<u></u>
Salinity ^b g/kg_sln	Chlorosit	y Treatment	a log ^a Observ	10 ⁴ s ^b S g-mol(1)/ 1 reddm ³	10 ³ mass ratio ^b g(1)/100 g sln	10 ⁶ mole fractior X 1
31.8	17.96	MF	-3.715	1.93	2.47	3.47
			-3.717	1.92	2.46	3.45
31.8	17.96	GFF	-3.713	1.94	2.48	3.49
			-3.712	1.94	2.49	3.49
31.9	18.00	CENT	-3.704	1.98	2.53	3.56
			-3.708	1.96	2.51	3.53
31.5	17.81	MF	-3.721	1.90	2.44	3.42
			-3.722	1.91	2.45	3.41
31.8	17.95	GFF	-3.719	1.90	2.43	3.44
			-3.722	1.91	2.45	3.41
31.7	17.72	MF	-3.715		2.47	3.45
			-3.716		2.465	3.46
31.5	17.80	GFF	-3.719		2.45	3.41
			-3.720		2.44	3.43
9.8	5.45	MF	-3.630		3.005	4.22
			-3.630	2.344	3.005	4.22
					(continued	1)
				INFORMATION		
METHOD/APPA	RATUS/PROCEDI	JRE:		SOURCE AND PURITY	OF MATERIALS:	
Detail given in reference (1). Saturated solutions were prepared by equilibrating excess naphthalene and salt solution in an ampoule with shaking for 24 hours. The filtered saturated solution was analyzed by a UV Spectrophotometer.		red alene e with tered	from Natural Seawa West Falmou	Hinton, Valpa Florida Atical reagent Mallinckrodt Ater: collected Ith, Buzzards Ba Ashapaquit Cree	raiso, grade d at ay, Quick	
		ſ	ESTIMATED ERROR:			
		Solubility ± 3% (Authors)				
				Temperature ±	0.03°C (Autho:	rs)
			ł	REFERENCES:		
					I.E.; Thorne, R Chem. <u>1967</u> , 71	

# COMPONENTS:

(1) Naphthalene; C₁₀H₈; [91-20-3]

(2) natural seawater

ORIGINAL MEASUREMENTS:

Gordon, J.E.; Thorne, R.L.

Geochim. Cosmochim. Acta <u>1967</u>, 31, 2433-43.

Experimental Values: (continued)

Salinity ^b g/kg sln	Chlorosity (°/)	<u>Treatment</u> ^a	log S Observed	10 [*] s ^b . g-mol(1)/ dm ³	10³ mass ratio ^b g(1)/100 q sln	10 ⁶ mole _b fraction X 1
9.8	5.45	GFF	-3.629	2.35	3.01	4.23
			-3.632	2.33	2.99	4.20

^aMF, membrane (0.45µ) filtered; GFF, glass fiber filtered; CENT, centrifuged

^bValues calculated by compiler.

Temperature = 24.91°C

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ [91-20-3]	Eganhouse, R.P.; Calder, J.A.
(2) Artificial seawater (ref 1)	Geochim. Cosmochim. Acta <u>1976</u> , 40 555-61.
	333-01.
VARIABLES:	PREPARED BY:
One temperature: 25.0°C	
Salinity: 35 g/kg sln	M. Kleinschmidt and W. Shiu
EXPERIMENTAL VALUES:	I
	the second to be
The solubility of naphthalene in sea	
22.0 mg/kg sln. The corresponding m	ass percent and mole fraction,
$x_1$ , calculated by the compilers are	2.20 x 10 $^{\circ}$ g(1)/100 g sln and
$3.18 \times 10^{-6}$ .	
Chambiant magnite for other coliciti	or are also reported
Graphical results for other saliniti	es are also reported.
(	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium flask: 1 L Erlen-	(1) analytical grade salts for artificial seawater solution,
meyer flask with ground glass stopper and sidearm tap at base	reagent grade.
plugged with glass wool. The	
mixtures were agitated 12+ hr at 215 rpm on a New Brunswick	water: doubly distilled
gyrotary shaker; a 24 hr station-	
ary equilibrium period followed.	
Hydrocarbons were extracted with doubly-distilled hexane 3 times;	
concentrated by evaporation, with	
losses checked against an internal standard.	ESTIMATED ERROR:
	temperature: ± 0.5°C
Analysis: gas chromatography	soly: ± 0.293 (95% confidence
	interval). REFERENCES:
	1. Lyman, J.; Fleming, R.H.;
	J. Mar. Res. <u>1940</u> , 3, 135.

COMPONENTS:	
	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Schwarz, F.P.
<pre>(2) Sodium chloride; NaCl;     [7647-14-5]</pre>	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water; H ₂ O; [7732-18-5]	
_	
VARIABLES:	PREPARED BY:
Temperature: 8.6-31.8°C	
Salinity: 30 g(2)/kg sln	W.Y. Shiu, D. Mackay
EXPERIMENTAL VALUES:	
EXPERIMENTAL VALUES:	
Solubility of naphthalene	in 0.5 g-mol(2)/dm ³
	$10^4 \text{ mol}(1)/\text{L sln}$
<u></u>	
8.6	0.84
11.1 14.0	0.92 1.09
17.1	1.23
20.0	1.37
23.0 25.0	1.58 1.73
31.8	2.22
<u> </u>	
3.13 x 10 ⁻⁶ .	
AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS;
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;
	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole %
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements.	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole % Sodium chloride: reagent grade
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements.	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 -
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight 1x1 cm quarts fluorescence	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight 1x1 cm quarts fluorescence cell containing 5 mL salt solution.	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 -
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight 1x1 cm quarts fluorescence	SOURCE AND PURITY OF MATERIALS; Naphthalene: purity > 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight 1x1 cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The Spectrofluorimeter em- ployed a ratio-photon counting mode where naphthalene concentration was	<pre>SOURCE AND PURITY OF MATERIALS: Naphthalene: purity &gt; 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.</pre>
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight 1x1 cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The Spectrofluorimeter em- ployed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence	SOURCE AND PURITY OF MATERIALS: Naphthalene: purity > 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The Spectrofluorimeter em- ployed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphtha-	<pre>SOURCE AND PURITY OF MATERIALS: Naphthalene: purity &gt; 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.</pre>
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The Spectrofluorimeter em- ployed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphtha- lene in ethanol therefore provide an	<pre>SOURCE AND PURITY OF MATERIALS: Naphthalene: purity &gt; 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.</pre> ESTIMATED ERROR: Solubility ± 3.3% (author) Temperature ± 0.1°C (author)
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The Spectrofluorimeter em- ployed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphtha-	<pre>SOURCE AND PURITY OF MATERIALS: Naphthalene: purity &gt; 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.</pre> ESTIMATED ERROR: Solubility ± 3.3% (author) Temperature ± 0.1°C (author)
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The Spectrofluorimeter em- ployed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphtha- lene in ethanol therefore provide an absolute solubility scale for the	<pre>SOURCE AND PURITY OF MATERIALS: Naphthalene: purity &gt; 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.</pre> ESTIMATED ERROR: Solubility ± 3.3% (author) Temperature ± 0.1°C (author)
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The Spectrofluorimeter em- ployed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphtha- lene in ethanol therefore provide an absolute solubility scale for the	<pre>SOURCE AND PURITY OF MATERIALS: Naphthalene: purity &gt; 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.</pre> ESTIMATED ERROR: Solubility ± 3.3% (author) Temperature ± 0.1°C (author)
METHOD/APPARATUS/PROCEDURE: The solubility of naphthalene in NaCl solution was determined by fluores- cence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The Spectrofluorimeter em- ployed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphtha- lene in ethanol therefore provide an absolute solubility scale for the	<pre>SOURCE AND PURITY OF MATERIALS: Naphthalene: purity &gt; 99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.</pre> ESTIMATED ERROR: Solubility ± 3.3% (author) Temperature ± 0.1°C (author)

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Components :	ORIGINAL MEASUREMENTS:			
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	May, W.E.; Wasik, S.P.; Freeman D.H.			
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.			
(3) Water; H ₂ O; [7732-18-5]				
VARIABLES:	PREPARED BY:			
One temperature: 25°C	W.Y. Chin and D. Vecher			
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay			
EXPERIMENTAL VALUES:				
The solubility of naphthalene in aqu	eous sodium chloride is			
reported in terms of the Setschenow	equation:			
$\log(S_{o}/S) = K_{s}C_{s}$				
where;				
S is the solubility	of (1) in water (mg/L)			
, v	f (1) in saline solution (mg/L)			
K_ is the Setschenow				
5				
5	on of sodium chloride (mol/L)			
evaluating the equation for S over t	he range of C _s 0-0.7 mol/L,			
$K_{s} = 0.213$ with $S_{o} = 31.69$ .				
The corresponding mass percent and mole fraction $x_1$ , at salinity =				
	1			
35 g(2)/kg sln calculated by the compilers are 2.29 x $10^{-3}$ g(1)/100 g sln				
and $3.29 \times 10^{-6}$ .				
AUXILIARY	INFORMATION			
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:			
A saturated solution of (1) was prepared by pumping salt water	(1) greater than 97% pure.			
through a "generation column" which	(2) reagent grade.			
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium			
saturated solution was extracted with an "extractor column" packed	permanganate-sodium hydroxide and passed through an XAD-2			
with a superficially porous bonded C ₁₈ stationary phase, then a water-	column.			
ačětonitrile solvent was passed				
through for extraction. The extract was introduced into a				
liquid chromatograph and the concen- tration of (1) was measured with a	ESTIMATED ERROR: temp ± 0.05°C			
UV detector.	K _s ± 0.001			
	s _o ± 0.23			
	REFERENCES :			

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1,2,4,5-Tetramethylbenzene; C₁₀H₁₄; [95-93-2]</pre>	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-244.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1,2,4,5-tetramethyl	contone in water at 25°C and at
system pressure was reported to be 3.4 mass per cent and mole fraction, $x_1$ , 6 3.48 x $10^{-4}$ g(l)/100 g sln and 4.67 x	calculated by the compiler are
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were car- ried out using a Hewlett-Packard Model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<ol> <li>Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>Distilled.</li> </ol>
	ESTIMATED ERROR:
	Temperature: ±1°C
	Solubility: ±0.28 mg(1)/kg(2)
	REFERENCES :
	AUF BAENCED ;

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COMPONENTS: (1) 1,2,4,5-Tetramethylbenzene; C ₁₀ H ₁₄ ; [95-93-2] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Krzyzanowska, T.; Szeliga, J. Nafta (Katowice), <u>1978</u> , 12, 413-7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	

EXPERIMENTAL VALUES:

The solubility of 1,2,4,5-tetramethylbenzene in water at 25°C was reported to be 3.48 mg(l)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 3.48 x 10⁻⁴ g(1)/100 g sln and 4.67 x 10⁻⁷.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

## AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	
Porasil column (70°C) and a flame	ESTIMATED ERROR:
ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	soly. 0.1 mg(1)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES:

COMPONENTS :	EVALUATOR:
<pre>(1) p-Cymene; C₁₀H₁₄; [99-87-5] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

## CRITICAL EVALUATION:

Quantitative solubility data for the p-cymene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1:	Quantitati	ve So	lubilit	y Studies	of
the p-	Cymene (1)	- Wate	er (2)	System	

Reference	T/K	Solubility	Method
Booth and Everson (ref 1)	298	(l) in (2)	volumetric
Englin et al. (ref 2)	283-303	(2) in (1)	analytical
Banerjee et al. (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

# 1. SOLUBILITY OF p-CYMENE (1) IN WATER (2)

Only two solubility values are available, both at 298K, but they are in poor agreement. The value of 0.04g(1)/100g sln reported by Booth and Everson (ref 1) is more than an order of magnitude greater than the value of  $2.34 \times 10^{-3} g(1)/100g$  sln reported by Banerjee *et al.* (ref 3). On the basis of comparison with similar systems the value of Banerjee *et al.* is more realistic.

### 2. SOLUBILITY OF WATER (2) IN p-CYMENE (1)

Only the values of Englin  $et \ al$ . (ref 2) are available and so no Critical Evaluation is possible. However, it may be noted that the data of Englin  $et \ al$ . are generally reliable at T < 300K but somewhat high at greater temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

## REFERENCES

- 1. Booth, H.S.; Everson, H.E. Ind. Eng. Chem. 1948, 40, 1491-3.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Environ. Sci. Technol. <u>1980</u>, 14, 1227-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Cymene; C ₁₀ H ₁₄ ; [99-87-5]	Booth, H.S.; Everson, H.E.
(2) Water; H ₂ O; [7732-18-5]	Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
VARIABLES:	DDEDADED NY
	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	I
The solubility of p-cymene in water a	
be 0.04 g(l)/100 mL(2). Assuming a :	
percentage and mole fraction, $x_{1}$ , cal	lculated by the compilers are
0.04 g(1)/100 g sln and 5 x $10^{-5}$ .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Stoppered Babcock tubes with neck	(1) source not specified;
graduated from 0 to 1.6 mL in steps of 0.02 mL were used. A	CP or highest commercial grade; used as received.
known volume of (2) (generally	
50 mL) was added to the tube in a constant-temperature water bath	(2) distilled.
and weighed quantities of (1)	
were added to this solution. The mixture was then shaken for 5	
minutes, returned to the bath for	
a minimum of 10 minutes and then centrifuged for 5 minutes. After	
this treatment, the volume of	ESTIMATED ERROR:
residue was determined directly.	soly. $\pm$ 0.1 mL(1)/100 mL(2).
	ma(2), 200 ma(2).
	REFERENCES :

COMPONENTS :			ORIGINAL MEASUREMENTS:		
<ol> <li>p-Cymene;</li> </ol>	C ₁₀ H ₁₄ ; [	99-87-6]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.		
(2) Water; H ₂ O; [7732-18-5]			Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.		
VARIABLES:		·	PREPARED BY:		
Temperature:	10-30°C		A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALU	ES:				
	Solu	bility of Wa	ter in p-Cymene		
	<u>t/°C</u> g	(2)/100 g s1	$n = \frac{10^3 x_2 (compiler)}{10^3 x_2 (compiler)}$		
	10 20	0.0223	1.66 2.27		
	30	0.0305 0.0415	3.08		
	·	AIIVTTTANU	INFORMATION		
METHOD/APPARATUS/	PROCEDURE .	AUXILIANI	SOURCE AND PURITY OF MATERIALS:		
Component (1)	was introdu	ced into a	(1) Not specified.		
thermostatted for 5 hr. with hydride was ac hydrogen volu the concentra evaluated.	h (2). Next ided and the me measured	, calcium evolving and hence	(2) Not specified.		
			ESTIMATED ERROR:		
			Not specified.		
			REFERENCES :		

	ORIGINAL MEASUREMENTS:
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Cymene; C ₁₀ H ₁₄ ; [99-87-5]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C.
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1980</u> , 14, 1227-9.
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of <i>p</i> -cymene in water w sln. Assuming a solution density of cent and mole fraction, $x_1$ , solubilit 2.34 x 10 ⁻³ g(1)/100 g sln and 3.13 x	1.00 kg/L the corresponding mass per . ies, calculated by the compiler, are
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Experiments were performed in sealed stainless steel centrifuge tubes. An	(1) Aldrich; purity not specified.
excess of $p$ -cymene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with con- stant or intermittent shaking. Equi- libration was generally complete with- in 1 week. The mixture was then cen- trifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C,	(2) Distilled.
following which aliquots of the solu- tion were removed for analysis by GC	ESTIMATED ERROR:
after exhaustive extraction with	Temperature: ±0.2°C
hexane. A HP 5370A (FID) instrument and a 3% OV-1 on Chromosorb W column was used. The entire procedure was	Solubility: ±3.1% rel. (represent- ing one std. dev.)
carried out at least twice for each Compound, and each analysis was also Conducted in duplicate.	REFERENCES :

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Diethylbenzene; C ₁₀ H ₁₄ ; [25340-17-4]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 0-50°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Wate: (isomer not	r in Diethylbenzene specified)
<u>t/°C</u> g(2)/100 g sln	<u>10³ x₂ (compiler)</u>
0 0.0159 10 0.0226 20 0.0319	1.57 2.23 3.15 4.25
30       0.0431         40       0.0574         50       0.0756	4.25 5.65 7.43
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was	(2) Not specified.
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:	EVALUATOR:
<pre>(1) tert-Butylbenzene; C₁₀H₁₄; [98-06-6]</pre> (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A. Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences Warszawa, Poland
	February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the tert-butylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Solubility Studies of the tert-Butylbenzene (1) - Water (2) System

Reference	<i>Т/</i> К	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Englin <i>et al</i> . (ref 2)	283-303	(2) in (1)	analytical
Sutton and Calder (ref 3)	298	(1) in (2)	GLC

The original data in all of the above publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF TERT-BUTYLBENZENE (1) IN WATER (2)

The two reported solubilities of *tert*-butylbenzene in water are in reasonable agreement (Table 2).

## TABLE 2: Tentative Value of the Solubility of tert-Butylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values 10 ³ g(1)/100g sln	"Best" value 10 ³ g(1)/100g sln	**
298	3.4 (ref 1), 2.95 (ref 3)	3.2 ± 0.2	4.3

 $\alpha$  Obtained by averaging,  $\sigma_n$  has no statistical significance.

2. SOLUBILITY OF WATER (2) IN TERT-BUTYLBENZENE (1)

As only the solubility values of Englin *et al*. (ref 2) are available no Critical Evaluation is possible. However, it may be noted that the data of Englin *et al*. are generally reliable at T < 300K but somewhat too high at greater temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

(continued next page)

COMPONENTS: (1) tert-Butylbenzene; C₁₀H₁₄; [98-06-6] (2) Water; H₂O; [7732-18-5] (2) Water; H₂O; [7732-18-5] (3) Water: H₂O; [7732-18-5] (4) Water: H₂O; [7732-18-5] (5) Water: H₂O; [7732-18-5] (5) Water: H₂O; [7732-18-5] (6) Water: H₂O; [7732-18-5] (7) Water: H₂O; [7) Water

CRITICAL EVALUATION: (continued)

REFERENCES

- 1. Andrews, L.J.; Keefer, T.M. J. Am. Chem. Soc. 1950, 72, 5034-7.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- 3. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) tert-Butylbenzene; C ₁₀ H ₁₄ ;	Andrews, L.J.; Keefer, R.M.		
[98-06-6]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.		
(2) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
One temperature: 25°C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
The solubility of tert-butylbenzene in water at 25°C was reported to be 0.0034 g(1)/100 g sln. The corresponding mole fraction, $x_1$ calculated by the compilers is 4.6 x 10 ⁻⁶ .			
*			
	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;		
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane	<ul> <li>(1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 167.8-168.0°C.</li> <li>(2) not specified.</li> </ul>		
blank on the Beckman spectrophoto- meter.	ESTIMATED ERROR:		
	not specified.		
	REFERENCES :		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) tert-Butylbenzene; C ₁₀ H ₁₄ ; [98-06-6]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.		
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.		
VARIABLES:	PREPARED BY:		
Temperature: 10-30°C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
Solubility of Water i	n tert-Butylbenzene		
$\frac{t/^{\circ}C}{g(2)/100 \text{ g sln}}$	$10^3 x_2$ (compiler)		
10 0.0205 20 0.0292	2.03		
20 0.0292 30 0.0389	2.88 3.83		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Component (1) was introduced into a	(1) Not specified.		
thermostatted flask and saturated for 5 hr. with (2). Next, calcium	(2) Not specified.		
hydride was added and the evolving hydrogen volume measured and hence			
the concentration of (2) in (1) was evaluated.			
evaluated.			
	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES :		
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) tert-Butylbenzene; C ₁₀ H ₁₄ ;	Sutton, C.; Calder, J.A.
[98-06-5]	J. Chem. Eng. Data 1975, 20,
	320-2.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
one temperature. 25 c	
EXPERIMENTAL VALUES:	1
The solubility of tert-butylbenzene	in water at 25°C was reported to be
29.5 mg(1)/kg(2). The corresponding	mass percent and mole fraction,
$x_1$ , calculated by the compilers are	0.00295 g(l)/100 g sln and
$3.95 \times 10^{-6}$ .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma-	(1) Aldrich Chemical Co. or Matheson Coleman and Bell
tography.	99+8.
	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.3 (the standard deviation of the mean for six replicates).
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:		
<pre>(1) tert-Butylbenzene; C₁₀H₁₄;</pre>	Sutton, C.; Calder, J.A.		
[98-06-6]	J. Chem. Eng. Data 1975, 20, 320-2.		
(2) Artificial seawater (ref 1)			
VARIABLES: One temperature: 25.0°C	PREPARED BY:		
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt and W. Shiu		
one satisfy: 54.5 g satts/kg sin	M. Riemschmidt and W. Shiu		
EXPERIMENTAL VALUES:			
The solubility of tert-butylbenzene :	in artificial seawater is reported to		
be 21.2 mg(l)/kg sln. The correspond	ding mass percent and mole fraction,		
$x_1$ calculated by the compiler are 2.2	$12 \times 10^{-3} g(1)/100 g sln and$		
2.92 x $10^{-6}$ assuming the artificial s			
	seawater composition of fer i.		
AUXILIARY	INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS;		
A test tube containing (1) was	(1) from either Aldrich Chemical		
placed in a flask containing (2)	Co. or Matheson Coleman and		
thus allowing for equilibration through the vapor phase. The	Bell, 99+% pure.		
saturated solution was extracted	(2) made from doubly distilled		
with hexane and analyzed by gas chromatography.	water and salts 99+% pure.		
chtomatography.			
	ESTIMATED ERROR:		
	temp. ± 0.1°C		
	soly. 0.3 (std. dev.)		
	REFERENCES:		
	1. Lyman, J.; Fleming, R.H.;		
	J. Mar. Res. <u>1940</u> , 3, 135.		

COMPONENTS:		EVALUATOR:	
(1) sec-Butylbenzene; C ₁₀ H ₁		A. Maczynski	
[135-98-8]	4'	Institute of Physical Chemistry of the Polish Academy of Sciences	
(2) Water; H ₂ O; [7732-18-5]		Warszawa, Poland.	
		November 1981	
CRITICAL EVALUATION:		•	
The solubility of sec-buty three works listed below:	lbenzene (1	) in water (2) has been reported in	
Authors	Method	T/K g(1)/100 g sln	
Andrews and Keefer (ref 1)	spectroph metric	oto- 298.15 0.0309	
Sutton and Calder (ref 3)	GLC	298.15 0.00176	
Krzyzanowska and Szeliga (ref 4)	GLC	298.15 0.00101	
The data of Andrews and Keefer seem to be high. The mean value of the remaining data is tentative.			
The solubility of water (2) one work listed below:	in sec-bu	tylbenzene (1) has been reported in	
Authors	Method	<u>T/K</u>	
Englin et al. (ref 2)	gasometr	ic 273.15-323.15	
Since these data are from one source only, they are regarded as tentative.			
SOLUBILITY OF se	C-BUTYLBEN TENTATIVE	ZENE (1) IN WATER (2) VALUE	
T/K	g(l)/100	g sln $\frac{x_1}{2}$	
298	0.00	14 $1.9 \times 10^{-6}$	
SOLUBILITY OF WATER (2) IN SEC-BUTYLBENZENE (1) TENTATIVE VALUES			
т/к	g(2)/100	g sln $\frac{x_2}{2}$	
283	0.02	0 0.0020	
293	0.02	9 0.0029	
303	0.03	9 0.0038	
REFERENCES			
l. Andrews, L.J.; Keefer,	R.M. J. A	mer. Chem. Soc. <u>1950</u> , 72, 5034-7.	
<ol> <li>Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.</li> </ol>			
3. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.			
4. Krzyzanowska, T.; Szeli	.ga, J. Na	fta (Katowice) <u>1978</u> , 12, 413-7.	

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) sec-Butylbenzene; C₁₀H₁₄; [135-98-8] (2) Water; H₂0; [7732-18-5]</pre>	Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
The solubility of sec-butylbenzene i reported to be 0.0309 g(1)/100 g slm The corresponding mole fraction, $x_1$ is 4.15 x $10^{-6}$ .	1.	
· · · · · · · · · · · · · · · · · · ·		
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:		
METHOD/APPARATUS/PROCEDURE: A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank	<ul> <li>(1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 175.0-175.8°C.</li> <li>(2) not specified.</li> </ul>	
on the Beckman spectrophotometer.	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) sec-Butylbenzene; C ₁₀ H ₁₄ ; [135-98-8]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	<i>Khim. Tekhnol. Topl. i Masel</i> <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of water	in sec-butylbenzene
t/°C g(2)/100 g s	sin x ₂ (compiler)
10 0.0226	0.00223
20 0.0317	0.00313
30 0.0426	0.00420
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(1) not specified.
for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was	(2) not specified.
evaluated.	
	ESTIMATED ERROR:
	Not specified,
	REFERENCES:
	-

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) sec-Butylbenzene; C ₁₀ H ₁₄ ;	Sutton, C.; Calder, J.A.
[135-98-8]	J. Chem. Eng. Data 1975, 20, 320-2.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of sec-butylbenzene in	n water at 25°C was reported to be
17.6 mg(1)/kg(2). The corresponding	mass percent and mole fraction,
$x_1$ , calculated by the compilers are (	
-	
$2.36 \times 10^{-6}$ .	
AUXILIARY	INFORMATION
ME THOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2)	(1) Aldrich Chemical Co. or
was determined by gas chroma-	Matheson Coleman and Bell 99+%.
tography.	
	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.2 (the standard deviation of the mean for six replicates).
1	REFERENCES:
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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) sec-Butylbenzene; C ₁₀ H ₁₄ ;	Krzyzanowska, T.; Szeliga, J.
[135-98-8]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of sec-butylbenzene in	n water at 25°C was reported
to be 10.1 mg(1)/kg(2).	
The corresponding mass percent and ma	ole fraction, $x_1$ , calculated
by compiler are 0.00101 g(l)/100 g s	ln and 1.36 x $10^{-6}$ .
METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in	(1) not specified.
(2) were prepared in two ways.	-
First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted	(2) not specified.
at 25°C. Second, the mixture of (1) and (2) as above was thermostatted	
at 70°C and then cooled to 25°C. The time required to obtain equilibrium	
was three weeks. The solubility of (1) in (2) was measured by glc. A	
Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh	
Porasil column (70°C) and a flame ionization detector was used. Sat-	ESTIMATED ERROR:
urated solutions of heptane in (2) were used as standard solutions.	soly. 0.3 mg(l)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES ;

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) sec-Butylbenzene; C ₁₀ H ₁₄ ;	Sutton, C.; Calder, J.A.		
[135-98-8]	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.		
(2) Artificial seawater (ref 1)			
VARIABLES:	DDEDADED NV.		
One temperature: 25.0°C	PREPARED BY:		
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt and W. Shiu		
EXPERIMENTAL VALUES:			
The solubility of sec-butylbenzene in	artificial seawater is reported		
to be 11.9 mg(1)/kg sln. The corresp	onding mass percent and mole fraction,		
$x_1$ calculated by the compiler are 1.1	$9 \times 10^{-3} q(1)/100 q sln and$		
-	1		
1.64 x $10^{-6}$ assuming the artificial s	eawater composition of ref 1.		
AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
A test tube containing (1) was	(1) from either Aldrich Chemical		
placed in a flask containing (2) thus allowing for equilibration	Co. or Matheson Coleman and Bell, 99+% pure.		
through the vapor phase. The			
saturated solution was extracted with hexane and analyzed by gas	(2) made from doubly distilled water and salts 99+% pure.		
chromatography.	water and suits 5516 part.		
	ESTIMATED ERROR:		
	temp. ± 0.1°C		
	soly. 0.2 (std. dev.)		
	REFERENCES :		
	<pre>1. Lyman, J.; Fleming, R.H.; J. Mar. Res. 1940, 3, 135.</pre>		

COMPONENTS: (1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. February 1986.
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CRITICAL EVALUATION:

Quantitative solubility data for the butylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

### TABLE 1: Solubility Studies of the Butylbenzene (1) - Water (2) System

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Klevens (ref 2)	298	(1) in (2)	spectrophotometric
Jones and Monk (ref 3)	298-308	(2) in (1)	radiotracer
Englin et al. (ref 4)	283-303	(2) in (1)	analytical
Massaldi and King (ref 5)	298	(1) in (2)	GLC
Sutton and Calder (ref 6)	298	(1) in (2)	GLC

The original data in all of the above publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

#### 1. SOLUBILITY OF BUTYLBENZENE (1) IN WATER (2)

The available data on the solubility of butylbenzene in water, all at 298K, are summarized in Table 2. The agreement is very poor with the reported values differing by almost two orders of magnitude which makes critical evaluation difficult. Fortunately, an independent estimation of the solubility can be made by extrapolation of the solubilities of the lower n-alkylbenzenes as a function of side chain length. This extrapolation predicts a value of  $1.7 \times 10^{-3}$  g(1)/100g sln. This value is quite close to the experimental values of Massaldi and King (ref 5) and Sutton and Calder (ref 6), the average of which is therefore suggested as the Tentative solubility of butylbenzene in water. The values of Andrews and Keefer (ref 1) and Klevens (ref 2) are correspondingly rejected.

COMPONENTS :	EVALUATOR:
2	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.
	February 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Solubility of Butylbenzene (1) in Water (2)

T/K	Solubilit	y values	
	Reported values	' "Best" values	$(\pm \sigma_n)^a$
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln	10 ⁶ x ₁
298	0.126 ^b (ref 1), 4.9 ^b (ref 2) 1.77 (ref 5), 1.18 (ref 6)	$1.5 \pm 0.3^{\circ}$	2.0

a Obtained by averaging but see text;  $\sigma_n$  has no statistical significance. b Rejected data, see text.

c Tentative value, see text.

#### 2. SOLUBILITY OF WATER (2) IN BUTYLBENZENE (1)

Although two publications report solubility data of water in butylbenzene, that of Jones and Monk (ref 3) is reported in v/v fractions and is thus excluded from consideration. The remaining data of Englin *et al.* (ref 4) cannot therefore be evaluated. However it may be noted that the values of Englin *et al.* are usually reliable at T < 300K but somewhat too high at greater temperatures. The interested user is referred to the relevant data sheet for the experimental values.

REFERENCES

- 1. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1950, 72, 5034-7.
- 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98.
- 3. Jones, J.R.; Monk, C.B. J. Chem. Soc. 1963, 2633-5.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- 5. Massaldi, H.A.; King, C.J. J. Chem. Eng. Data <u>1973</u>, 18, 393-7.
- 6. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.

COMPONENTE	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. 1950, 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of butylbenzene in wat to be 0.000126 g(1)/100 g sln.	er at 25°C was reported
The corresponding mole fraction, $x_1$ , is 1.69 x 10 ⁻⁷ .	calculated by the compilers
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was	<pre>(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. range 182.0-183.0°C.</pre>
withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered	(2) not specified.
Erlenmeyer flask. Next, the absorb- ance of the hexane phase was meas- ured against a hexane blank on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Butylbenzene; C₁₀H₁₄; [104-51-8] Klevens, H.B. J. Phys. Chem. <u>1950</u>, 54, 283-98. (2) Water; H₂O; [7732-18-5] VARIABLES: PREPARED BY: Temperature: 25°C M.C. Haulait-Pirson EXPERIMENTAL VALUES: The solubility of butylbenzene in water at 25°C was reported to be 0.05 g(1)  $L^{-1}$  sln and 0.00037 mol(1)  $L^{-1}$  sln. Assuming that 1.00 kg sln = 1.00 L sln the mass percentage and mole fraction  $x_1$ calculated by the compilers are 0.005 g(1)/100 g sln and 6.7 x  $10^{-6}$ . AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The solubility of (1) in (2) was determined by shaking small amounts (1) not specified. of (1) in 1 liter of (2) for as long (2) not specified. as three months. Aliquots were removed and concentrations determined by spectra. ESTIMATED ERROR: not specified. **REFERENCES:** 

	t
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8]	Jones, J.R.; Monk, C.B.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Soc. <u>1963</u> , 2633-35.
VARIABLES:	PREPARED BY:
Temperature: 25-35°C	A. Maczynski, Z. Maczynska and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of wat	cer in butylbenzene
<i>t</i> /°C 10	) ⁴ mL(2)/mL(1)
25	3.5
30	4.1
35	4.9
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass-stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mc/mL), decanted, a 5-mL aliquot reshaken for 4 hrs. with 5 mL H ₂ O in a 10-mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintilla- tion counter. The two-stage process eliminates quenching effects (due to solvent) on the scintillator.	<pre>SOURCE AND PURITY OF MATERIALS:    (1) laboratory grade dried over CaCl₂ and fractionally distilled.    (2) not specified.    ESTIMATED ERROR: soly. ± 5% to ± 1% (average deviation)    REFERENCES: 1. Vogel Practical Organic</pre>

2	o	n
2	o	2

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8] (2) Water; H ₂ 0; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2, mator, m ₂ 0, [,,or 10 0]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Wate	r in Butylbenzene
<u>t/°C</u> g(2)/100 g s1	n $10^3 x_2$ (compiler)
10 0.0234	1.74
20 0.0331 30 0.0448	2.46 3.33
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hr. with (2). Next, calcium	(2) Not specified.
hydride was added and the evolving	(2) Not specified.
hydrogen volume measured and hence the concentration of (2) in (1) was	
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	-
	REFERENCES :
	REFERENCES :
	REFERENCES:
	REFERENCES :
	REFERENCES:
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8]	Massaldi, H.A.; King, C.J.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1973</u> , 18, 393-7.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of butylbenzene in wat 1.32 x 10 ⁻⁴ mol(1) dm ⁻³ sln. The corresponding mass percent and mo by the compilers are 0.00177 g(1)/100	ble fraction, $x_1$ , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A technique based on head-space analysis by gas-liquid chromato- graphy was developed to determine solubilities of sparingly soluble organics. Saturated solutions need not be prepared in advance whereby phase separation problems are avoided, nor have liquid samples to be analyzed. This method is ver- satile enough to allow determina- tions provided that the pure vapor	<ol> <li>Matheson Coleman and Bell Co., highest purity; used as received.</li> <li>not specified.</li> </ol>
pressure of the substances is known. The gas chromatograph was a Varian	ESTIMATED ERROR:
Aerograph Model 1740 with a flame ionization detector.	temp. ± 0.05°C
	REFERENCES:

COMPONENTS: (1) Butylbenzene; C₁₀H₁₄; [104-51-8]

(2) Water; H₂O; [7732-18-5]

# Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.

ORIGINAL MEASUREMENTS:

VARIABLES: One temperature:	PREPARED BY: A. Maczynski and Z. Maczynska

# EXPERIMENTAL VALUES:

The solubility of butylbenzene in water at 25°C was reported to be 11.8 mg(1)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compilers are 0.00118 g(1)/100 g sln and  $1.58 \times 10^{-6}$ .

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	<ul> <li>(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.</li> </ul>
	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 0.1°C soly. 0.1 mg(1)/kg(2)
	(the standard deviation of the
	mean for six replicates) REFERENCES:

	285
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8]	Sutton, C.; Calder, J.A.
(2) Artificial seawater (ref 1)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2
VARIABLES:	PREPARED BY:
One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	M. Kleinschmidt and W. Shiu
EXPERIMENTAL VALUES:	
The solubility of butylbenzene in an	
7.09 mg(l)/kg sln. The correspondin	lg mass percent and mole fraction, 09 x $10^{-4}$ g(l)/kg sln and 9.76 x $10^{-7}$
-	
assuming the artificial seawater com	position of ref 1.
······································	
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A test tube containing (1) was	SOURCE AND PURITY OF MATERIALS: (1) from either Aldrich Chemical
placed in a flask containing (2) thus allowing for equilibration	Co. or Matheson Coleman and Bell, 99+% pure.
through the vapor phase. The saturated solution was extracted	(2) made from doubly distilled
with hexane and analyzed by gas chromatography.	water and salts 99+% pure.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.07 (std. dev.)
	REFERENCES:
	<pre>l. Lyman, J.; Fleming, R.H.; J. Mar. Res. <u>1940</u>, 3, 135.</pre>

COMPONENTS:		ORIGINAL MEASUREMENTS:
<pre>(1) (+)-(R)-P-Mentha-1,8-diene (d-Limonene); C₁₀H₁₆; [5989-27-5] (2) Water; H₂O; [7732-18-5]</pre> Massaldi, H.A.; King, C.J. J. Chem. Eng. Data <u>1973</u> , 18, 39		Massaldi, H.A.; King, C.J. J. Chem. Eng. Data <u>1973</u> , 18, 393-7.
VARIABLES:		PREPARED BY:
Temperature: 0-25°C		A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:		
Solubi	lity of d-lim	onene in water
$t/^{\circ}$ C mg(1) L sln 10 ⁴	mol(l) L sl	n $10^{3}g(1)/100g \ sln \ (compiler) \ 10^{6}x_{1}$
0 9.7	0.708	0.97 1.3
5 10.4	0.767	1.04 1.4
25 13.8	1.013	1.38 1.8
		THEORMATION
NETHOD ADDADATUS ADDOCEDURE	AUXILIARI	INFORMATION
METHOD/APPARATUS/PROCEDURE: A technique based on hea analysis by gas-liquid c graphy was developed to solubilities of sparingl organics. Saturated sol not be prepared in advan phase separation problem avoided, nor have liquid be analyzed. This metho satile enough to allow d tions provided that the pressure of the substance The gas chromatograph wa Aerograph Model 1740 wit ionization detector.	chromato- determine y soluble utions need to whereby as are samples to od is ver- letermina- pure vapor ces is known.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Matheson Coleman and Bell Co., highest purity; kept under N2 atmosphere at -2°C in a dark container; used as received. (2) not specified. (2) not specified. ESTIMATED ERROR: temp. ± 0.05°C</pre>
		REFERENCES :

COMPONENTS: (1) Bicyclo[4.4.0]decane (deca- hydronaphthalene; decalin); $C_{10}H_{18}$ ; [91-17-8] (2) Water; $H_2O$ ; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
2	April 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the decalin (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of theDecalin (1) - Water (2) System

Reference	T/K	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	volumetric
Englin <i>et al</i> . (ref 2)	293-313	(2) in (1)	analytical
Price (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

#### 1. SOLUBILITY OF DECALIN (1) IN WATER (2)

The solubility of decalin in water has been reported only at 298K (Table 1). However, the datum of Booth and Everson (ref 1) in v/v fraction, is only an order of magnitude result and must thus be excluded. Since this leaves only the single datum of 8.89 x  $10^{-5}g(1)/100g \sin(x_1 = 1.16 \times 10^{-7})$  of Price (ref 3) no Critical Evaluation is possible. Nevertheless, it may be noted that the solubility values reported by Price are usually reliable although for the higher hydrocarbons his results are often about 20% (relative) lower than Recommended values.

# 2. SOLUBILITY OF WATER (2) IN DECALIN (1)

As only the data of Englin *et al*. (ref 2) over the range 293-313K are available no Critical Evaluation is possible. However, it may be noted that the data of Englin *et al*. are generally reliable when T < 300K but are somewhat high at higher temperatures. The interested user is referred to the relevant data sheet for the experimental values.

#### REFERENCES

- 1. Booth, H.S.; Everson, H.E. Ind. Eng. Chem. <u>1948</u>, 40, 1491-3.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- 3. Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u>, 60, 213-44.

200	_
COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Bicyclo[4.4.0]decane (Decahydro- naphthalene); C₁₀H₁₈; [91-17-8]</pre>	Booth, H.S.; Everson, H. Ind. Eng. Chem. <u>1948</u> , 4, 1491-3.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of bicyclo[4.4.0]decand be <0.02 mL(1)/100 mL(2).	e in water at 25°C was reported to
A similar result was reported for (1) xylenesulfonate.	in 40.0% (w/w?) aqueous sodium
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.03 mL. An excess of solute was added and the mixture allowed to come to equi- librium in a constant temperature bath then centrifuged. The amount of solute dissolved was determined by subtracting the undissolved solute, measured directly in the	(1) "Highest grade commercial sam- ple available"; no other details given.
	(2) Distilled.
tube, from the total added.	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Bicyclo[4.4.0]decane (deca- hydronaphthalene; decalin) C₁₀H₁₈; [91-17-8]</pre>	Englin, B.A.; Plate, A.F.; Tugoluko V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-40°C	A. Maczynski and M.C. Haulait-Pirso
EXPERIMENTAL VALUES:	I
Colubility of Water i	n Bicyclo[4.4.0]decane
Solubility of water 1	$10^4 x_2$
<u>t/°C</u> <u>g(2)/100</u>	
20 0.00	
30 0.01 40 0.01	
AUXILIARY	INFORMATION
	INFORMATION SOURCE AND PURITY OF MATERIALS:
ETHOD/APPARATUS/PROCEDURE:	
ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a hermostatted flask and saturated for 5 hours with (2). Next, calcium ydride was added and the evolving ydrogen volume measured and hence he concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS:
ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a hermostatted flask and saturated for 5 hours with (2). Next, calcium aydride was added and the evolving bydrogen volume measured and hence the concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS: (1) Not specified.
ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a chermostatted flask and saturated for 5 hours with (2). Next, calcium aydride was added and the evolving aydrogen volume measured and hence the concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS: (1) Not specified.
AUXILIARY ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium bydride was added and the evolving bydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified.
ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a chermostatted flask and saturated for 5 hours with (2). Next, calcium aydride was added and the evolving aydrogen volume measured and hence the concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR:
ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a hermostatted flask and saturated for 5 hours with (2). Next, calcium aydride was added and the evolving bydrogen volume measured and hence the concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified.
ETHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a hermostatted flask and saturated for 5 hours with (2). Next, calcium aydride was added and the evolving bydrogen volume measured and hence the concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified.

COMPONENTS :	ORIGINAL MEASUREMENTS:	
<ul> <li>(1) Bicyclo[4.4.0]decane (deca- hydronaphthalene;decalin); C₁₀H₁₈; [91-17-8]</li> <li>(2) Water; H₂O; [7732-18-5]</li> </ul>	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of bicyclo[4.4.0]decane in water at 25°C and at system pressure was reported to be 0.889 mg(1)/kg(2). The corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are 8.89 x 10 ⁻⁵ g(1)/100 g sln and 1.16 x 10 ⁻⁷ .		
AUXILIARY	INFORMATION	
ME THOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<ol> <li>Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>distilled.</li> </ol>	
	ESTIMATED ERROR: temp. ± 1°C soly. ± 0.031 mg(1)/kg(2) REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Pentylcyclopentane; C ₁₀ H ₂₀ ;	Price, L.C.	
	Am. Assoc. Petrol. Geol. Bull.	
(2) Water; H ₂ O; [7732-18-5]	<u>1976</u> , 60, 213-44.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:	······································	
The solubility of pentylcyclopentane in water at 25°C and at system pressure was reported to be 0.115 mg(1)/kg(2). The corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler was 1.15 x 10 ⁻⁵ g(1)/100 g sin and 1.5 x 10 ⁻⁸ .		
AUXILIARY METHOD /APPARATUS / PROCEDURE :	INFORMATION SOURCE AND PURITY OF MATERIALS:	
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were car- ried out by GLC using a Hewlett- Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<ul> <li>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.</li> <li>(2) Distilled.</li> </ul>	
	ESTIMATED ERROR: Temp. ±1°C Soly. ±0.011 mg(1)/kg(2)	
	REFERENCES:	

292 COMPONENTS: ORIGINAL MEASUREMENTS: (1) 1-Decene; C₁₀H₂₀; [872-05-9] Natarajan, G.S.; Venkatachalam, K.A. (2) Water; H₂O; [7732-18-5] J. Chem. Eng. Data. 1972, 17, 328-9. VARIABLES: PREPARED BY: Temperature: 15-25°C M.C. Haulait-Pirson and G.T. Hefter EXPERIMENTAL VALUES: Solubility of 1-decene in 0.001 mol/L HNO3 sln.  $10^3 g(1)/100 g sln^b$  $10^{6} x_{1}$ 10⁵ mol/L sln^a t/°C g(l)/100 g sln (compiler) (compiler) 15 8.2 1.1 1.5 20 6.1 0.85 1.1 25 4.1 0.57 0.73 ^a Uncertainties stated to be "standard deviations from mean". ^b Assuming a solution density of 1.00 g mL⁻¹ at all temperatures. Compilers' note: Although the data have not been measured in pure water the low concentration of the added acid is unlikely to cause the olefin solubility to differ markedly from that in pure water. Further solubility data are given in the paper for 0.05 and 0.1 mol/L HC1. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 15 mL of the aqueous medium was (1) BDH: 99% equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted (2) Not specified. glass burette. After settling (judged) visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures. ESTIMATED ERROR: Temp. ±0.05 K Soly. see Table above. **REFERENCES:** 

	293	
COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) 2,7-Dimethyloctane; C ₁₀ H ₂₂ ; [1072-16-8]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.	
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.	
VARIABLES:	PREPARED BY:	
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
Solubility of Water	in 2,7-Dimethyloctane	
<u>t/°C</u> <u>g(2)/10</u>	$\begin{array}{c} 10^4 \ x_2 \\ 0 \ g \ sln \end{array} \qquad (compiler)$	
10 0.00		
20 0.00 30 0.01		
AUXILIARY	INFORMATION	
METHOD /APPARATUS / PROCEDURE :		
Component (1) was introduced into a	SOURCE AND PURITY OF MATERIALS: (1) Not specified.	
thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(2) Not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS: (1) Decane; C₁₀H₂₂; [124-18-5] (2) Water; H₂O; [7732-18-5] EVALUATOR: M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

CRITICAL EVALUATION:

Quantitative solubility data for the decane (1) - water (2) system have been reported in the publications listed in Table 1.

		·····	
Reference	T/K	Solubility	Method
Baker (ref 1,2)	298	(1) in (2)	radiotracer
Schatzberg (ref 3)	298,313	(2) in (1)	Karl Fischer
Franks (ref 4)	298	(1) in (2)	GLC
McAuliffe (ref 5)	298	(1) in (2)	GLC
Krasnoshchekova and Gubergrits (ref 7)	298	(1) in (2)	GLC
Mackay <i>et al</i> . (ref 8)	_ ^a	(1) in (2)	GLC
Namiot et al. (ref 9)	423 <b>-</b> 583 ^b	(2) in (1)	vapliq.equil.
Skripka (ref 10)	398-563 ^b	(2) in (1)	vapliq.equil.
Becke and Quitzsch (ref 11)	293	mutual	refractometric

a Not specified but probably 298.15K.

b Pressure also varied 1-78 MPa.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition, Roof (ref 6) has reported a three phase critical point of unknown composition at 569K and 9.6 MPa. For convenience further discussion of this system will be divided into two parts.

## 1. SOLUBILITY OF DECANE (1) IN WATER (2)

The available data on the solubility of decane in water are summarized in Table 2 with the following exceptions. The value of Baker in ref 2 is quoted in v/v terms and is therefore excluded from consideration (however it is equivalent to that reported by the same author in ref 1). The values of Mackay *et al.* (ref 8) are rejected not only because the measurement temperature was unspecified but also because the authors themselves regard their solubility values below  $2 \times 10^{-3}$ g(1)/100g sln as potentially unreliable because of emulsion or colloid formation. The value of McAuliffe (ref 5) is also rejected because it is very much higher than all other reported values.

Agreement among the remaining values (Table 2) is not good enough to enable any of the "Best" values to be Recommended.

(continued next page)

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# TABLE 1: Quantitative Solubility Studies of<br/>the Decane (1) - Water (2) System

r	· · · · · · · · · · · · · · · · · · ·		
COMPONENTS:		EVALUATOR:	
(1) Decan	e; C ₁₀ H ₂₂ ; [124-18-5]	M.C. Haulait-Pirson, Depart Chemistry, University of Le	
(2) Water	; H ₂ O; [7732-18-5]	Belgium.	
	2	G.T. Hefter, School of Math and Physical Sciences, Murd	loch
		University, Perth, W.A., Au	stralia.
CRITICAL EVA	LUATION: (continued)		
		lung of the Colubility of	
	TABLE 2: Tentative Va     Decane (1) in	lues of the Solubility of h Water (2)	
T/K			
	Reported values	"Best" values	$(\pm \sigma_n)^{\alpha}$
	10 ⁶ g(1)/100g sln	10 ⁶ g(1)/100g sln	10 ⁵ x ₁
293	1.98 (ref 11)	2	2.5
298	l.6 (ref l), l.98 (ref 4),	1.5 ± 0.5	1.9
	0.87 (ref 7)		
a Obtained	l by averaging; on has no sta	tistical significance.	
	11		I
2. SOLUB	ILITY OF WATER (2) IN DECANE	: (1)	
	eric pressure the only avail		-
	ecane are those of Schatzber		
	These data are listed in Ta e regarded as order of magni		nent and
oun only b	e regarded as order or magni		
At higher	temperatures and pressure on	ly the data of Skripka and o	co-workers
	are available and so no Cri		
	user is referred to the rel	evant Data Sheets for the ex	<periment-< td=""></periment-<>
al values.			
	TABLE 3: Approximate	Solubility Values of	
		Decane (1)	
T/K		d values ^a	
	10 ² g(2)/100g sln	$10^{3} x_{2}$	
293	2.92 (ref 11)	2.3	
298	0.72 (ref 3)	0.6	
313	1.36 (ref 3)	1.1	
a Values co	onsidered as order-of-magnit	ude data only, see text.	
REFERENCES			
1. Baker, No.4,	, E.G. Am. Chem. Soc., Div. C61-8.	Petrol. Chem., Preprints 1	<u>.958</u> , 3,
	, E.G. Science <u>1959</u> , 129,		
3. Schat:	zberg, P. J. Phys. Chem. 1	<u>963</u> , 67, 776-9.	
		(continued ne	xt page)

COMPONENTS: EVALUATOR: M.C. Haulait-Pirson, Department of (1) Decane; C₁₀H₂₂; [124-18-5] Chemistry, University of Leuven, Belgium. (2) Water; H₂O; [7732-18-5] G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. CRITICAL EVALUATION: (continued) REFERENCES (continued) Franks, F. Nature 1966, 210, 87-8. 4. McAuliffe, C. Science 1969, 163, 478-9. 5. Roof, J.G. J. Chem. Eng. Data 1970, 15, 301-3. 6.

- Krasnoshchekova, P.Y.; Gubergrits, M.Y. Neftekhimiya <u>1973</u>, 13, 885-7.
- Mackay, D.; Shiu, M.W.; Wolkoff, A.W. Water Quality Parameters, ASTM STP 573, <u>1975</u>, 251-8.
- 9. Namiot, A.Y.; Skripka, V.G.; Lotler, Y.G. Zh. Fiz. Khim. <u>1976</u>, 50, 2718; Deposited doc. 1976; VINITI 1213-76.
- Skripka, V.G. Tr. Vses. Neftegazov. Nauch-Issled. Inst. <u>1976</u>, 61, 139-51.
- 11. Becke, A.; Quitzsch, G. Chem. Techn. 1977, 29, 49-51.

COMPONENTS:	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Baker, E.G.
(2) Water; H ₂ O; [7732-18-5]	Am. Chem. Soc., Div. Petrol. Chem., Preprints <u>1958</u> , 3, N°4, C61-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	· · · · · · · · · · · · · · · · · · ·
The solubility of decane-1-C ¹⁴ in wa to be 16 x 10 ⁻⁹ g(1)/g(2). The corresponding mole fraction, cal- is $x_1 = 2.0 \times 10^{-9}$ .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	
- INOD/REFARATUS/FROCEDURE:	SOURCE AND PURITY OF MATERIALS;
Carbon-14 labeled (1) was used as radioactive tracer. The technique of preparing a satu- rated aqueous solution of (1) by ultrafiltration of a (1)-(2) dis- persion has been described in ref 1. A Packard Tri-Carb Liquid Scintilla- tion Spectrometer was used to detect the radioactive (1) dissolved in (2).	<ul> <li>(1) Nuclear Instrument and Chemical Corporation; used as received.</li> <li>(2) distilled.</li> </ul>
	ESTIMATED ERROR:
	soly. 20% (standard deviation from 17 replicate runs).
	REFERENCES :
	<ol> <li>Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints- Symposia <u>1956</u>, 1, N°2, 5.</li> </ol>

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Baker, E.G.
(2) Water; H ₂ O; [7732-18-5]	Science <u>1959</u> , 129, 871-4.
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
	-
EXPERIMENTAL VALUES:	
The solubility of decane in water at	25°C was reported to be
The solubility of decade in water at $22 \times 10^{-7}$ mL(1)/100 mL(2).	ZJ C was reported to be
	ſ
	······
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
not specified.	not specified.
	ESTIMATED ERROR:
	1
	not specified.
	REFERENCES:

	299		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Schatzberg, P.		
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.		
VARIABLES:	PREPARED BY:		
Temperature: 25-40°C	M.C. Haulait-Pirson		
-			
EXPERIMENTAL VALUES:			
Solubility of wat	ter in decane		
t/°C mg(2)/	'kg sln ^x 2		
25 72	$2^{a}$ 5.7 x 10 ⁻⁴		
40 136	$5^{b}$ 10.7 x 10 ⁻⁴		
a.b	,,,		
a,b See "Estimated Error"			
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
(1) was saturated by storing over a	(1) Phillips Petroleum Co.; research		
layer of (2) in a brown glass bottle without any agitation. The bottle	grade; 99.43 mole%; passed repeatedly through a column		
was sealed with serum cap and com- pletely submerged in the water-bath	of silica gel until no absorp- tion occurred in the 220 to		
for 7 days. A 20-mL sample was withdrawn with a silicone-hydro- phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly ESTIMATED ERROR:			
		in the presence of methanol to a "dead-stop" end-point using a	temp. ± 0.02°C
		Beckman KF3 automatic titrimeter.	<pre>soly. a) 0-6%; b) 0-2% (deviations from the mean)</pre>
	REFERENCES:		

HWW 2-U

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Decane; C₁₀H₂₂; [124-18-5] Franks, F. Nature (London) 1966, 210, 87-8. (2) Water; H₂O; [7732-18-5] VARIABLES: PREPARED BY: F. Kapuku One temperature: 25°C EXPERIMENTAL VALUES: The solubility of decane in water at 25°C was reported to be in mole fraction  $x_1 = 2.5 \times 10^{-9}$ . The corresponding mass percent calculated by the compiler is  $1.98 \times 10^{-6} g(1)/100 g sln.$ AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD /APPARATUS / PROCEDURE : The analysis was performed by gas (1) Fluka; purum grade; purity > 97% (chromatographic liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 ml of the analysis). aqueous phase was injected into the (2) not specified. fractionator fitted to the chromatographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations. ESTIMATED ERROR: soly. ± 12% **REFERENCES:** 

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	McAuliffe, C.	
(2) Water; H ₂ O; [7732-18-5]	Science <u>1969</u> , 163, 478-9.	
VARIABLES:		
	PREPARED BY:	
One temperature: 25°C	F. Kapuku	
EXPERIMENTAL VALUES:		
The solubility of decane in water at 25°C was reported to be 0.052 mg(1)/kg(2). The corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are 5.2 x $10^{-6}$ g(1)/100 g sln and 6.58 x $10^{-9}$ .		
	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
(1) was equilibrated with (2). Glass	(1) not specified.	
vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaken for 2 minutes. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.	(2) distilled.	
	ESTIMATED ERROR:	
	soly. ± 0.0043 mg(l)/kg(2)	
	REFERENCES:	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Water; H ₂ 0; [7732-18-5]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u> , 13, 885-7.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski
EXPERIMENTAL VALUES: The solubility of decane in water at $x_1 = 1.1 \times 10^{-9}$ . The corresponding mass percent calcu 8.7 x 10 ⁻⁷ g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigor- ously stirred magnetically for 10- 12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliguots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.	<pre>SOURCE AND PURITY OF MATERIALS: (1) source not specified; CP reagent; purity not specified. (2) distilled. (2) distilled. ESTIMATED ERROR: not specified. REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Decane; C₁₀H₂₂; [124-18-5] (2) Water; H₂0; [7732-18-5]</pre>	<pre>Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. 1975, 573, 251-8.</pre>
VARIABLES: not specified	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported two different values for the solubility of decane in water: 0.182 and 1.22 mg(1)dm⁻³ sln. With the assumption of a solution density of 1.00 g cm⁻³, the corresponding mass percents calculated by the compiler, are 0.0000182 and 0.000122 g(1)/100 g sln and the corresponding mole fractions,  $x_1$ , are 2.3 x 10⁻⁸ and 1.6 x 10⁻⁷ respectively.

AUXILIARY INFOR	MATION		
	AUXILIARY INFORMATION		
<ul> <li>(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equili- brations it is possible to calculate the amount of (1) in the original sample.</li> </ul>	EE AND PURITY OF MATERIALS: not specified. not specified. MATED ERROR: estimated. WENCES:		

MENTS: .; Skripka, V.G.; .G. n. <u>1976</u> , <i>50</i> , 2718 <u>doc.</u> 1976, 3-76.
g(2)/100 g sln (compiler)
0.36
1.31
2.39
4.01
7.87
11.4
16.3
0.38
0.93
1.60
2.54
3.82
5.45
7.99
12.06
TY OF MATERIALS:
ot specified; CP used as received.
d.
d.
R.G.; Skripka, V.G.; 'u.A. Zh. Fiz. Khim. 2170.

				30
COMPONENTS:			ORIGINAL MEASUREMEN	TS:
	ne; C ₁₀ H ₂₂ ; [124-1		Skripka, V.G. Tr. Vses. Nefteg Inst. <u>1976</u> , 6	gazov. Nauch. Issled.
(2) Water	с, H ₂ O; [7732-18-5	]		
			Sultanov, R.G.; Zh. Fiz. Khim.	<u>1973</u> , <i>47</i> , 1035.
VARIABLES:			PREPARED BY:	
	ire: 225-290°C 2.9-78.5 MPa		A. Maczynski	
EXPERIMENTA	L VALUES: Solubi	lity of wat	er in decane	
t/°C	<i>p</i> /kg cm ⁻²	p/MPa (compil	er) ^x 2	g(2)/100 g sln (compiler)
225	30	2.9	0.162	2.39
	50 70	4.9 6.9	0.157 0.153	2.30 2.28
	100	9.8	0.148	2.15
	150 200	14.7 19.6	0.138 0.132	1.99 1.89
	250	24.5	0.124	1.76
	300 400	29.4 39.2	0.118 0.108	1.67 1.51
	500	49.0	0.102	1.42
	600	58.8 68.6	0.098 0.095	1.36 1.31
	700 800	78.5	0.094	1.30
250	50	4.9 6.9	0.255 0.248	4.15 4.01
	70 100	9.8	0.240	3.84
	150 200	14.7 19.6	0.226 0.213	3.56 3.31
	250	24.5	0.200	3.07
	300 400	29.4 39.2	0.190 0.168	2.88 2.49
	500	49.0	0.158	2.32
	600 700	58.8 68.6	0.153 0.151	2.24 2.20
	800	78.5	0.148	2.15
			INFORMATION	
METHOD/APPAR	ATUS/PROCEDURE:		SOURCE AND PURITY OF	MATERIALS:
described	imental technique in ref l. No det in the paper.		reagent grad	pecified, chemical e; purity not sed as received.
			(2) distilled.	
			ESTIMATED ERROR:	
			not specified.	
			REFERENCES:	
			<ol> <li>Sultanov, R.G. Namiot, A.Yu. <u>1971</u>, 4, 6.</li> </ol>	.; Skripka, V.G.; Gazov. Prom.
				· · · · · · · · · · · · · · · · · · ·

	; C ₁₀ H ₂₂ ; [124-18-5] H ₂ O; [7732-18-5]	Tr. Vset Inst. Sultanov		pka, V.G.
t/°C	$p/kg \text{ cm}^{-2}$	p/MPa (compiler)	<i>x</i> ²	g(2)/100 g sln (compiler)
275	70	6.9	0.404	7.90
	100	9.8	0.385	7.34
	150	14.7	0.353	6.46
	200	19.6	0.220	5.62
	250	24.5	0.293	4.98
	300	29.4	0.272	4.52
	400	39.2	0.246	3.97
	500	49.0	0.231	3.66
	600	58.8	0.217	3.39
	700	68.6	0.204	3.14
	800	78.5	0.197	3.08
290	100	9.8	0.580	14.88
	150	14.7	0.417	8.30
	200	19.6	0.392	7.54
	250	24.5	0.371	6.95
	300	29.4	0.350	6.38
	400	39.2	0.318	5.57
	500	49.0	0.291	4.94
	600	58.8	0.270	4.47
	700	68.6	0.253	4.11
	800	78.5	0.243	3.90

COMPONENTS:	
	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Becke, A.; Quitzsch, G.
(2) Water; H ₂ O; [7732-18-5]	Chem. Techn. <u>1977</u> , 29, 49-51.
VARIABLES:	PREPARED BY:
One temperature: 20°C	P.L. Huyskens and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of decane in water at	20°C was reported to be in
mole fraction, $x_1 = 2.5 \times 10^{-9}$ . The	corresponding mass percent,
calculated by the compiler, is 1.976	$x 10^{-6}$ g(l)/l00 g sln. The
solubility of water in decane at 20°C	, was reported to be in mole
fraction, $x_2 = 2.3 \times 10^{-3}$ . The corre	
culated by the compiler, is 0.0292 g	2)/100 g sln.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The refractometric and the Karl-	not specified.
Fischer dead-stop titration methods were used.	
No more details are given in the paper.	
Faber.	
	ESTIMATED ERROR:
	soly. 0.05-1% for (1) in (2) 0.3-1.3% for (2) in (1)
	REFERENCES:
ĺ	

COMPONENTS :	EVALUATOR:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
1	December 1982

CRITICAL EVALUATION:

The solubility of decane (1) in seawater (2) has been reported in two works:

Authors	Method	т/к 	Salinity g salts/kg sln	g(1)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	298	6	$8.7 \times 10^{-6}$
Freegarde <i>et al</i> . (ref 2)	GLC	?	?	$1.5 \times 10^{-5}$

Because temperature and salinity are not specified, the data of Freegarde  $et \ al$ . are rejected. The value of Krasnoshchekova and Gubergrits is considered doubtful since it is greater than the tentative value for the solubility of decane in pure water at 298 K.

SOLUBILITY OF DECANE (1) IN SEAWATER (2) DOUBTFUL VALUE

T/K	g salts/kg sln	g(l)/100 g sln
		·····
298	6	$8.7 \times 10^{-6}$

Ĺ

#### REFERENCES

- Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u>, 13, 885-8.
- 2. Freegarde, M.; Hatchard, C.G.; Parker, C.A. Lab. Pract. <u>1971</u>, 20, 35-40.

	30
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Freegarde, M.; Hatchard, C.G.; Parker, C.A.
(2) Seawater (composition not specified)	Lab Pract. 1971, 20, 35-40.
-	
VARIABLES:	PREPARED BY:
Temperature, pressure, salinity not given.	M. Kleinschmidt and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of decane was reporte	d to be 0.15 mg/L. The
Corresponding mass percent and mole	
the compilers are $1.5 \times 10^{-5}$ g(1)/10	
assuming a solution density of 1.02	
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
None given except that analysis was done using gas chromatography.	not given.
	ESTIMATED ERROR: not specified.
	REFERENCES :

310 COMPONENTS: ORIGINAL MEASUREMENTS: Krasnoshchekova, R.Ya.; (1) Decane; C₁₀H₂₂; [124-18-5] Gubergrits, M.Ya. (2) Seawater Neftekhimiya 1973, 13, 885-8. VARIABLES: PREPARED BY: One temperature: 25°C M. Kleinschmidt Salinity: 6 g/kg sln **EXPERIMENTAL VALUES:** The solubility of decane in seawater was reported to be  $8.7 \times 10^{-6}$  g(1)/100 g sln. and the corresponding mole fraction,  $x_1 = 1.1 \times 10^{-8}$ .

## AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: (1) "chemically pure" A saturated solution was prepared by vigorously stirring hydrocarbon (2) distilled water plus salt (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solumixture. tion was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated. ESTIMATED ERROR: not specified. **REFERENCES:**

COMPONENTS:	EVALUATOR:
<pre>(1) 1-Methylnaphthalene; C₁₁H₁₀; [90-12-0]</pre> (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 1-methylnaphthalene (1) - water (2) system have been reported in the publications listed in Table 1.

# TABLE 1: Quantitative Solubility Studies of the1-Methylnaphthalene (1) - Water (2) System

Reference	T/K	Solubility	Method
Englin $et \ al.$ (ref 1)	273-323	(2) in (1)	analytical
Eganhouse and Calder (ref 2)	298	(1) in (2)	GLC
Mackay and Shiu (ref 3)	298	(1) in (2)	spectrofluorometric
Schwarz and Wasik (ref 4)	283-298	(1) in (2)	spectrofluorometric
Schwarz (ref 5)	282-305	(1) in (2)	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

For further convenience further discussion of this system is divided into two parts.

1. SOLUBILITY OF 1-METHYLNAPHTHALENE (1) IN WATER (2)

All the available data on the solubility of 1-methylnaphthalene in water are summarized in Table 1 with the exception of those of Schwarz and Wasik which have been rejected as they are much more scattered than those in the Paper by Schwarz (ref 5). There are insufficient data to warrant plotting.

At 298K, the only temperature where comparison is possible, the data are in excellent agreement and the average value can be Recommended. At other temperatures only the data of Schwarz (ref 5) are available and must thus be considered as Tentative only.

TABLE 2:Recommended (R) and Tentative Values of the Solubility of1-Methylnaphthalene (1) in Water (2)

T/K	Solubil	ity values	
	Reported values ^a 10 ³ g(1)/100g sln	"Best" values ( $\pm \sigma_n$ 10 ³ g(1)/100g sln 10 ⁶ x	
283			T
203	2.05* (ref 5) 2.56* (ref 5)	2.1     2.7       2.6     3.3	
	2.50 (IEI 5)	(Table 2 continued next pa	qe)

 COMPONENTS:
 EVALUATOR:

 (1) 1-Methylnaphthalene, C₁₁H₁₀;
 G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch

 (2) Water; H₂O; [7732-18-5]
 University, Perth, W.A., Australia.

 February 1986.

 CRITICAL EVALUATION: (continued)

 Table 2 (continued)

 T/K
 Solubility values Reported values^a

 "Best" values (± gn)^b

 $\frac{10^{3} g(1)/100 g \sin 10^{3} g(1)/100 g \sin 10^{6} x_{1}}{2.98}$ 298
2.58 (ref 2), 2.85 (ref 3)
2.95* (ref 5)
303
3.35* (ref 5)
3.4
4.3

*a* Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original data. *b* Obtained by averaging where relevant;  $\sigma_n$  has no statistical significance.

2. SOLUBILITY OF WATER (2) IN 1-METHYLNAPHTHALENE (1)

As only the data of Englin *et al*. (ref 1) are available on the solubility of water in 1-methylnaphthalene no Critical Evaluation is possible. However, it may be noted that the solubility values of Englin *et al*. are generally reliable for T < 300K but are larger than Recommended values at higher temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

REFERENCES

- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- 2. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.
- 3. Mackay, D.; Shui, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.
- 4. Schwarz, F.P.; Wasik, S.P. J. Chem. Eng. Data 1977, 22, 270-3.
- 5. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Methylnaphthalene; C₁₁H₁₀; [90-12-0]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 0-50°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Water	in l-Methylnaphthalene
<u>t/°C</u> <u>g(2)/10</u>	$10^{3} x_{2}$ 0 g sln (compiler)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	282     2.22       377     2.97       485     3.82       519     4.87
AUXILIARY	INFORMATION

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Methylnaphthalene; C₁₁H₁₀;</pre>	Eganhouse, R.P.; Calder, J.A.
[90-12-0]	Geochim. Cosmochim. Acta <u>1976</u> ,
(2) Water; H ₂ 0; [7732-18-5]	40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

#### EXPERIMENTAL VALUES:

The solubility of 1-methylnaphthalene in water at 25°C was reported to be 25.8 mg(1)/kg(2) and 1.81 x  $10^{-4}$  mol(1) L (2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 2.58 x  $10^{-3}$  g(1)/100 g sln and 3.27 x  $10^{-6}$ .

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<ol> <li>source not specified; analytical grade; used as received; no impurities by glc.</li> <li>doubly distilled; free of trace organics.</li> </ol>		
	ESTIMATED ERROR:		
	temp. ± 0.5°C soly. ± 1.2 mg(1)/kg(2) (from eight determinations)		
	REFERENCES:		

COMPONENTS :	
(1) 1-Methylnaphthalene; C ₁₁ H ₁₀ ;	ORIGINAL MEASUREMENTS: Mackay, D.; Shiu, W.Y.
[90-12-0]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1-methylnaphthalene to be 28.5 mg(1) dm ⁻³ sln and $x_1 = 3$ . The corresponding mass percent calcul	$.55 \times 10^{-6}$ .
is $0.00285 g(1)/100 g sln.$	lated by the compiler
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2)	(1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently	Kodak, or K and K Laboratories, commercial highest grade;
settled at 25°C for at least 48 hrs.	used as received.
Then the saturated solution was decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	
funnel. After shaking for 2 hrs.	
the cyclohexane extract was removed for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. $\pm$ 0.3 mg(1) dm ⁻³ sln
in the paper.	(maximum deviation from several determinations).
	REFERENCES:

316			
COMPONENTS :	*** ***	ORIGINAL MEASUREMENTS:	
(1) l-Methylna	phthalene; C ₁₁ H ₁₀ ;	Schwarz, F.P.	
[90-12-0]		J. Chem. Eng. Data 19	9 <u>77</u> , 22, 273-7.
(2) Water; H ₂ O	; [7732-18-5]		
VARIABLES:		PREPARED BY:	
Temperature: 8	.6-31.7°C	A. Maczynski	
		L <u></u>	
EXPERIMENTAL VALUES:			
	Solubility of 1-methylr	_	<i>c</i>
t/°C	10 ⁴ mol(1) L ⁻¹	10 ³ g(1)/100 g sln (compiler)	10 ⁶ x1 (compiler)
8.6	1.40 ± 0.03	1.99	2.52
14.0	1.59 ± 0.03	2.26	2.86
17.1	1.61 ± 0.03	2.29	2.90
20.0	1.78 ± 0.02	2.53	3.21
23.0	$1.94 \pm 0.02$	2.76	3.49
25.0	$2.11 \pm 0.07$	3.00	3.80
26.1 29.2	$2.14 \pm 0.02$ $2.34 \pm 0.05$	3.04 3.33	3.85 4.21
31.7	$2.54 \pm 0.05$ $2.55 \pm 0.04$	3.27	4.21
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/P	ROCEDURE:	SOURCE AND PURITY OF MATERI	ALS;
Two methods we	re used.	(1) source not specif:	
	lubility of (1) in (2)	than 99.9 mole%, I used as received.	oy dro!
measurements a	from UV absorption nd was used as a	(2) distilled over KMm	NO4 and NaOH
standard at ot At other tempe	her temperatures. ratures the	and passed through column.	n a Sephadex
	etry method was used.		
	orescence cells		
	of the aqueous n excess of (1) were		
	st 72 h in a water oved, quickly wiped	ESTIMATED ERROR:	
	in the fluorimeter.	temp. ± 0.1°C	
		soly. see above	
		REFERENCES:	
J		1	

COMPONENTS :		ORIGINAL MEASUREMENTS:		
(1) 1-Methylnaphthalene; C ₁₁ H ₁₀ ;		Schwarz, F.P.; Wasik, S.P.		
		J. Chem. Eng. Data <u>1977</u> , 22, 270-3.		
(2) Water;	H ₂ 0; [7732-18-5]			
VARIABLES:		PREPARED BY:		
Temperatur	ce: 10-25°C	A. Maczynski		
EXPERIMENTAL	VALUES:			
	Solubility of 1-methyl	naphthalene in water		
t/°C	$10^4 \text{ mol}(1) \text{ L}^{-1}$	10 ³ g(1)/100 g sln (compiler)	10 ⁶ x1 (compiler)	
10	1.6	2.3	2.9	
14	2.0	2.8	3.6	
20	2.0	2.8	3.6	
25	2.1	3.0	3.8	
	AUXILIARY	INFORMATION		
METHOD/APPARA	AUXILIARY TUS/PROCEDURE:	INFORMATION SOURCE AND FURITY OF MATERI	ALS :	
The solubi determined Since the (2) are to	TUS/PROCEDURE: lity of (1) in (2) was from its absorbance. concentration of (1) in so low to determine its	SOURCE AND PURITY OF MATERI (1) Chemical Samples ( Columbus, Ohio; b) 99.9 mole%.	Co., etter than	
The solubi determined Since the (2) are to extinction the absorp performed the satura	TUS/PROCEDURE: lity of (1) in (2) was from its absorbance. concentration of (1) in	SOURCE AND PURITY OF MATERI (1) Chemical Samples Columbus, Ohio; b	Co., etter than nO4 and passed	
The solubi determined Since the (2) are to extinction the absorp performed the satura	TUS/PROCEDURE: .lity of (1) in (2) was l from its absorbance. concentration of (1) in po low to determine its a coefficient accurately, otion measurements were on measured volumes of ated solutions diluted	<pre>SOURCE AND PURITY OF MATERI (1) Chemical Samples Columbus, Ohio; b 99.9 mole%. (2) distilled from KMM</pre>	Co., etter than nO4 and passed	
The solubi determined Since the (2) are to extinction the absorp performed the satura	TUS/PROCEDURE: .lity of (1) in (2) was l from its absorbance. concentration of (1) in po low to determine its a coefficient accurately, otion measurements were on measured volumes of ated solutions diluted	<ul> <li>SOURCE AND PURITY OF MATERI</li> <li>(1) Chemical Samples (Columbus, Ohio; b)</li> <li>99.9 mole%.</li> <li>(2) distilled from KMI through a Sephade:</li> </ul>	Co., etter than nO ₄ and passed x column.	
The solubi determined Since the (2) are to extinction the absorp performed the satura	TUS/PROCEDURE: .lity of (1) in (2) was l from its absorbance. concentration of (1) in po low to determine its a coefficient accurately, otion measurements were on measured volumes of ated solutions diluted	<ul> <li>SOURCE AND PURITY OF MATERI</li> <li>(1) Chemical Samples of Columbus, Ohio; bo 99.9 mole%.</li> <li>(2) distilled from KM through a Sephade:</li> </ul>	Co., etter than nO ₄ and passed x column.	
The solubi determined Since the (2) are to extinction the absorp performed the satura	TUS/PROCEDURE: .lity of (1) in (2) was l from its absorbance. concentration of (1) in po low to determine its a coefficient accurately, otion measurements were on measured volumes of ated solutions diluted	<pre>SOURCE AND PURITY OF MATERI (1) Chemical Samples ( Columbus, Ohio; b) 99.9 mole%. (2) distilled from KM through a Sephader ESTIMATED ERROR: temp. ± 0.1°C soly. ± 2 x 10⁻⁵ mol(</pre>	Co., etter than nO ₄ and passed x column.	
The solubi determined Since the (2) are to extinction the absorp performed the satura	TUS/PROCEDURE: .lity of (1) in (2) was l from its absorbance. concentration of (1) in po low to determine its a coefficient accurately, otion measurements were on measured volumes of ated solutions diluted	<pre>SOURCE AND PURITY OF MATERI (1) Chemical Samples ( Columbus, Ohio; b) 99.9 mole%. (2) distilled from KM through a Sephader ESTIMATED ERROR: temp. ± 0.1°C soly. ± 2 x 10⁻⁵ mol(</pre>	Co., etter than nO ₄ and passed x column.	

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COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Methylnaphthalene; C₁₁H₁₀; [90-12-0]</pre>	Schwarz, F.P.
<pre>(2) Sodium chloride; NaCl; [7647-14-5]</pre>	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES: Temperature: 8.1-28.5°C	PREPARED BY: W.Y. Shiu, D. Mackay
Salinity: 30 g(2)/kg sln	W.I. SHIU, D. Mackay
EXPERIMENTAL VALUES:	
Solubility of 1-methylnaph	thalene in 0.5 mol(2)/L
<u>t/°C</u>	$10^4 \text{ mol}(1)/\text{L sln}$
8.1	1.23
11.1	1.35
15.5 17.4	1.49 1.53
18.2	1.54
20.7	1.54
23.3	1.63
25.0 28.5	1.69 1.81
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of 1-methylnaphthalene in NaCl solution was determined by	1-Methylnaphthalene: purity > 99%,
fluorescence and UV absorption mea- surements. In the fluorescence	Sodium chloride: reagent grade,
method, saturated solution was pre- pared by adding excess amount of	Ethanol: reagent grade,
l-methylnaphthalene to an air-tight l x l cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent inten-	Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column.
sity was measured at 350 and 320 nm.	ESTIMATED ERROR:
The Spectrofluorimeter employed a ratio-photon counting mode where 1-methylnaphthalene concentration	Solubility ± 3.6% (author) Temperature ± 0.1°C (author)
was linearly related to the fluores- cence signal. The UV method was used to obtain the absorptivity of l-methylnaphthalene in ethanol there- fore provide an absolute solubility scale for the fluorescence method.	REFERENCES :

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COMPONENTS: (1) 2-Methylnaphthalene; C ₁₁ H ₁₀ ; [91-57-6] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.			
	December 1985.			
CRITICAL EVALUATION: Quantitative solubility data for 2-methylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data appear to				
have been reported on the solubility (	of water in 2-methylnaphthalene.			
TABLE 1: Quantitative Solubility Studies of         2-Methylnaphthalene (1) in Water (2)				
Reference	T/K Method			
Eganhouse and Calder (ref 1)	298 GLC			
Mackay and Shiu (ref 2)	298 spectrofluorometric			
-	-			
excellent agreement and thus the mean           TABLE 2:         Recommended (R)         V           2-Methylnaphthalene         2	Value of the Solubility of			
	bility values			
Reported values	"Best" value $(\pm \sigma_n)^a$			
10 ³ g(1)/100g sln	10 ³ g(1)/100g sln 10 ⁶ x ₁			
298 2.46 (ref 1), 2.54 (ref 2)	2.50 ± 0.04 (R) 3.2 (R)			
$a$ Calculated by averaging; $\sigma_n$ has no statistical significance.				
REFERENCES				
<ol> <li>Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.</li> </ol>				
2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u> , 22, 399-402.				

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Methylnaphthalene; C₁₁H₁₀; [91-57-6]</pre>	Eganhouse, R.P.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

#### EXPERIMENTAL VALUES:

The solubility of 2-methylnaphthalene in water at 25°C was reported to be 24.6 mg(l)/kg(2) and 1.72 x  $10^{-4}$  mol(l) dm⁻³(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 2.46 x  $10^{-3}$  g(1)/100 g sln and 3.12 x  $10^{-6}$ .

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) source not specified; analytical grade; used as received; no impurities by glc.</li> <li>(2) doubly distilled; free of trace organics.</li> </ul>	
	ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.5 mg (1)/kg(2) (from eight determinations) REFERENCES:	

COMPONENTS:	
	ORIGINAL MEASUREMENTS:
(1) 2-Methylnaphthalene; C ₁₁ H ₁₀ ;	Mackay, D.; Shiu, W.Y.
[91-57-6]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
one competature. 25 c	M.C. Madiait-Filson
EXPERIMENTAL VALUES:	
The colubility of 2 methodrout the long	in water at 25% was repeated
The solubility of 2-methylnaphthalene to be 25.4 mg(1) dm ⁻³ sln and $x_1 = 3$ .	
$\begin{bmatrix} co \ be \ 25.4 \ mg(1) \ dm \\ \end{bmatrix} = 3.$	22 x 10 .
The corresponding mass percent calcul	ated by the compiler
is 0.00254 g(1)/100 g sln.	
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AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2)	(1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL	Kodak, or K and K Laboratories,
flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	commercial highest grade; used as received.
Then the saturated solution was	
decanted and filtered and 50-100 mL extracted with approximately 5 mL	(2) doubly distilled.
of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American	
Instruments Ltd.) was used for analysis. Many details are given	ESTIMATED ERROR:
in the paper.	soly. ± 0.2 mg(1) dm ⁻³ sln (maximum deviation from several
	determinations).
	PEEDENCIA
	REFERENCES:

NENTS:		

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Ethyl-1,3,5-trimethylbenzene; C₁₁H₁₆; [3982-67-0]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-40°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Water in 2-Et	hyl-1,3,5-trimethylbenzene
<u>t/°C</u> g(2)/100 g sl	$n = 10^3 x_2 (compiler)$
20         0.0259           30         0.0350           40         0.0461	2.13 2.87 3.78
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	<ul><li>(1) Not specified.</li><li>(2) Not specified.</li></ul>
	ESTIMATED ERROR: Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) tert-Pentylbenzene; C ₁₁ H ₁₆ ;	Andrews, L.J.; Keefer, R.M.
[2049-95-8]	J. Am. Chem. Soc., <u>1950</u> , 72,
(2) Water; H ₂ O; [7732-18-5]	5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of tert-pentylbenzene	e in water at 25°C was reported
to be 0.00105 g(1)/100 g sln.	-
The corresponding mole fraction, $x_1$ ,	calculated by the compilers
is 1.27 x 10 ⁻⁶ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was	(1) Eastman Kodak Co. white label;
rotated twenty hours in a constant temperature bath at 25°C. A sample	<pre>fractionally distilled; b.p. range 188.0-189.0°C.</pre>
(5-20 mL) of the aqueous phase was	_
withdrawn and extracted with a measured volume of hexane (10-50 mL)	(2) not specified.
by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorb-	
ance of the hexane phase was meas-	
ured against a hexane blank on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

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COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 3-Methylbicyclo[4.4.0]decane (2-methyldecalin); C₁₁H₂₀; [2958-76-1]</pre> (2) Water; H ₂ 0; [7732-18-5]	Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints <u>1958</u> , 3, N°4, C61-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2-methyl- $C^{14}$ decaling reported to be 40.6 x 10 ⁻⁹ g(1)/g(2).	in water at 25°C was
The corresponding mass percentage and the compiler are $4.06 \times 10^{-6}$ g(1)/100	mole fraction, $x_1$ , calculated by g sln and 4.82 x $10^{-9}$ .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Carbon-14 labeled (1) was used as tracer. The technique of preparing a saturated aqueous solu- tion of (1) by ultrafiltration of a	<ul> <li>(1) Nuclear Instrument and Chemical Corporation; used as received.</li> <li>(2) distilled.</li> </ul>
(1)-(2) dispersion has been described in ref 1. A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dis- solved in (2).	
	ESTIMATED ERROR:
	soly. 20% (standard deviation from 17 replicate runs).
	REFERENCES :
	<pre>LIBAKES: 1. Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints- Symposia 1956, 1, N°2, 5.</pre>

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Components :	ORIGINAL MEASUREMENTS:
(1) Hexylcyclopentane; C ₁₁ H ₂₂ ; [4457-00-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	L
Solubility of Water	in Hexylcyclopentane
+ / ⁹ C ~ ~ (2) (1)	$10^4 x_2$
<u>t/°C</u> <u>g(2)/10</u>	
30 0.0	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hours with (2). Next calcium	(2) Not specified.
hydride was added and the evolving hydrogen volume measured and hence	-
the concentration of (2) in (1) was	
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	not specified.
	REFERENCES:

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COMPONENTS: (1) Undecane; C₁₁H₂₄; [1120-21-4] (2) Water; H₂O; [7732-18-5] (2) Water; H₂O; [7732-18-5] (3) Water: H₂O; [7732-18-5] (4) Water: H₂O; [7732-18-5] (5) Water: H₂O; [7732-18-5] (5) Water: H₂O; [7732-18-5] (5) Water: H₂O; [7732-18-5] (6) Water: H₂O; [7732-18-5] (7) Water: H₂O; [7) Water: H

December 1985.

CRITICAL EVALUATION:

Quantitative solubility data for the system undecane (1) - water (2) have been reported in the publications listed in Table 1.

TABLE 1:	Quantitat:	ive Soluk	oility	Studies of
the Un	decane (1)	- Water	(2) Sy	ystem

Reference	T/K	Solubility	Method
Schatzberg (ref 1)	298,313	(2) in (1)	Karl Fischer
McAuliffe (ref 2)	298	(1) in (2)	GLC
Krasnoshchekova and Gubergrits (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF UNDECANE (1) IN WATER (2)

The available data for the solubility of undecane in water are listed in Table 2.

TABLE 2: Solubility Values of Undecane (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value	
	10 ⁷ g(1)/100g sln	10 ⁷ g(1)/100g sln	10 ¹⁰ x1
298	4.4 (ref 2), 3.6 (ref 3)	$4.0 \pm 0.4^{a}$	4.6 ^{<i>a</i>}

a Order of magnitude only, see text; obtained by averaging.

Although the agreement between the two studies (ref 2,3) is very good considering the very low solubility involved, both values are very much lower than expected from an extrapolation of *n*-alkane solubilities. This may be due (ref 2) to micelle formation. The available data must therefore be considered as Doubtful. The extrapolated value of 1.4 x  $10^{-6}$  g(1)/100g sln ( $x_1 = 1.6 \times 10^{-10}$ ) may be more realistic.

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(continued next page)

December 1985.
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CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN UNDECANE (1)

As only one publication (ref 1) reports solubility data for water in undecane no Critical Evaluation is possible. However, it may be noted that the data of Schatzberg (ref 1) are generally reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

REFERENCES

1. Schatzberg, P. J. Phys. Chem. <u>1963</u>, 67, 776-9.

2. McAuliffe, C. Science <u>1969</u>, 163, 478-9.

 Krasnoshchekova, P.Y.; Gubergrits, M.Y. Neftekhimiya <u>1973</u>, 13, 885-7.

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Undecane; C ₁₁ H ₂₄ ; [1120-21-4]	Schatzberg, P.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.
VARIABLES:	PREPARED BY:
Temperature: 25-40°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of wate	r in undecane
t/°C mg(2)/	kg sln ^x 2
25 69	a $6.0 \times 10^{-4}$
40 130	
a,b See "Estimated Error"	
See Estimated Error"	
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION
METHOD/APPAKAIUS/FROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was saturated by storing over a	(1) Phillips Petroleum Co.; research
layer of (2) in a brown glass bottle without any agitation. The bottle	grade; 99.33 mole%; passed repeatedly through a column
was sealed with serum cap and com-	of silica gel until no absorp-
pletely submerged in the water-bath for 7 days. A 20-mL sample was	tion occurred in the 220 to 340 nm spectral range.
withdrawn with a silicone-hydro- phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted	(2) distilled and deionized.
to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly	FOTTMATED EDDODA
in the presence of methanol to a	ESTIMATED ERROR: temp. ± 0.02°C
"dead-stop" end-point using a Beckman KF3 automatic titrimeter.	<pre>soly. a) 0-6%; b) 0-2% (deviations     from the mean)</pre>
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Undecane; C ₁₁ H ₂₄ ; [1120-21-4]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Science <u>1969</u> , 163, 478-9.
-	
VARIABLES :	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of undecane in water a 0.0044 mg(1)/kg(2). The corresponding mass percent and maby the compiler are 4.4 x 10 ⁻⁷ g(1)/1	ble fraction, $x_1$ , calculated
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
(1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaken for 2 minutes. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.	(2) distilled.
	ESTIMATED ERROR:
	soly. $\pm$ 0.0018 mg(1)/kg(2)
	REFERENCES :

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Undecane; C ₁₁ H ₂₄ ; [1120-21-4]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya.
(2) Water; H ₂ O; [7732-18-5]	_
2	Neftekhimiya <u>1973</u> , 13, 885-7.
VARIABLES:	
	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of undecane in water a $x_1 = 4.10 \times 10^{-10}$ . The corresponding mass percent calcul 3.6 x $10^{-7}$ g(1)/100 g sln.	
AUXILIARY	INFORMATION
ME THOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
	sound had token of initering,
A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigor- ously stirred magnetically for 10- 12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliguots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air,	<ul> <li>(1) source not specified; CP reagent; purity not specified.</li> <li>(2) distilled.</li> </ul>
and the (1)-saturated air was analyzed by glc.	ESTIMATED ERROR:
	not specified.
	REFERENCES:

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Components :	ORIGINAL MEASUREMENTS:
(1) Undecane; C ₁₁ H ₂₄ ; [1120-21-4]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.
(2) Seawater	Neftekhimiya <u>1973</u> , 13, 885-8.
	_
VARIABLES:	PREPARED BY:
One temperature: 25°C	PREPARED DI:
Salinity: 6 g/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of undecane in seawat	er was reported to be
$1.0 \times 10^{-6}$ g(1)/100 g sln. and the c	orresponding mole fraction,
$x_1 = 1.2 \times 10^{-9}$ .	
T	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution was prepared by vigorously stirring hydrocarbon	(1) "chemically pure"
(1) in seawater (2) for 10-12 hrs.	(2) distilled water plus salt mixture.
in a flask placed in a temperature controlled bath. A sample of solu-	mixture.
tion was then transferred to a closed flask with head space volume	
equal to solution volume. Hydro- carbon concentration in the head	
space was determined by gas chroma-	
tography and the corresponding solution concentration calculated.	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS :	EVALUATOR:
<pre>(1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	March 1986.

CRITICAL EVALUATION:

Quantitative solubility data for acenaphthene (1) in water (2) have been reported in the publications listed in Table 1. No data appear to have been reported for the solubility of water in acenaphthene.

	Quantitative S			
0	f Acenaphthene	(1) in	Water	(2)

Reference	<i>Т/</i> К	Method
Wauchope and Getzen (ref 1)	273-348	spectrophotometric
Eganhouse and Calder (ref 2)	298	GLC
Mackay and Shiu (ref 3)	298	spectrofluorometric
Banerjee <i>et al</i> . (ref 4)	298	radiotracer
Rossi and Thomas (ref 5)	298	GLC, spectrophotometric
Rossi and momas (ref 5)	250	dic, spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

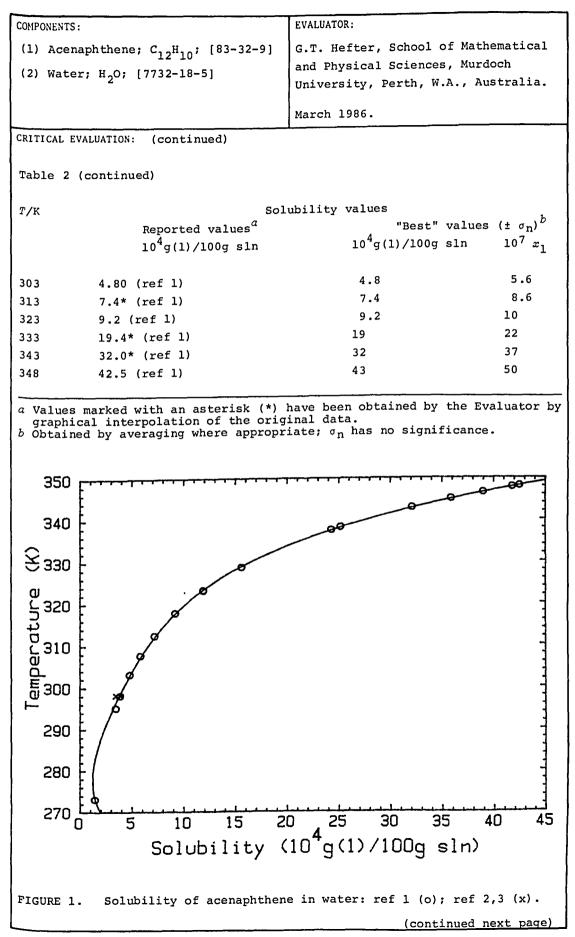
At 298K, the only temperature where comparison is possible (Table 1), the data of Wauchope and Getzen (ref 1), Eganhouse and Calder (ref 2) and Mackay and Shiu (ref 3) are in excellent agreement. The values of Banerjee *et al.* (ref 4) and Rossi and Thomas (ref 5) are respectively very much higher and lower and are therefore rejected.

At other temperatures only the data of Wauchope and Getzen (ref 1) are available and must therefore be regarded as Tentative values.

The solubility values of acenaphthene in water are summarized in Table 2 and plotted in Figure 1.

TABLE	2:	Recommended					Values	for
		Acenap	hth	ene	(l) in Wat	er (2)		

T/K	Solubilit	ty values	
	Reported values ^a	"Best" values	
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln	10 ⁷ x ₁
273	1.45 (ref 1)	1.5	1.8
293	3.2* (ref 1)	3.2	3.7
298	3.88 (ref 1), 3.47 (ref 2), 3.93 (ref 3)	3.8 ± 0.2 (R)	4.4( <i>R</i> )
1		(Table 2 continued n	ext page)



COMPONENTS: (1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Water; H₂O; [7732-18-5] Water; H₂O; [7732-18-5] Warch 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

- 1. Wauchope, R.D.; Getzen, F.W. J. Chem. Eng. Data 1972, 17, 38-41.
- 2. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40, 555-61.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.
- Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Environ. Sci. Technol. <u>1980</u>, 14, 1227-9.
- 5. Rossi, S.S.; Thomas, W.H. Environ. Sci. Technol. 1981, 15, 715-6.

COMPONEN	TS:		IORIG	INAL MEASUREMENTS:	
		[83-32-91		chope, R.D.; Getzen,	F.W.
<pre>(1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Water; H₂O; [7732-18-5]</pre>			J. Chem. Eng. Data 1972, 17,		
(2) water; $n_20; [7/32-16-5]$			8-41.	_/ _//	
VARIABLES:			PREP	ARED BY:	
Temper	ature: 0-75°C		A. Maczynski		
Elimantica					
CAPERIME	NTAL VALUES:	ty of acena	phth	ene in water	
		-			
t/°C [·]		smoothed wi		$10^4$ g(1)/100 g sln	$10^{7}x_{1}$
	experiment	(std_dev)		(compiler)	(compiler)
0.0 22.0	2 57	1.45(0. 3.46	04)	1.45 3.46	1.69 4.04
22.0	3.57	3.46 3.88(0.	07)	3.46	4.04
30.0	4.76, 4.60, 4.72	4.80	- • •	4.80	5.61
34.5	6.00, 5.68, 5.73	5.83		5.83	6.81
39.3 44.7	6.8, 7.1, 7.0	7.2 9.2		7.2 9.2	8.4 10.7
50.0	9.4, 9.4, 9.3	11.9(0.1	)	11.9	13.9
50.1	12.5, 12.4, 12.4	11.9	•1	11.9	13.9
55.6	15.8, 16.3, 15.9	15.6		15.6	18.2
64.5	25.9, 27.8	24.3		24.3 25.2	28.4
65.2 69.8	23.7, 23.4, 22.8 30.1, 34.3, 33.6	25.2 32.1		32.1	29.4 37.5
_	35.2	35.9		35.9	41.9
73.4	39.1, 40.1	39.0		39.0	45.6
74.7 75.0	40.8, 39.3	41.8 42.5(0.7	、	41.8 42.5	48.8 49.7
<b></b>					
	· · · · · · · · · · · · · · · · · · ·	AUXILIARY	INFOR		
MERUOD (15		AUXILIARI			
	PPARATUS/PROCEDURE:		i i	E AND PURITY OF MATERIALS	
	mately 20 g of (1) w		(1)	Baker reagent; recry	stallized
	of three 250-mL gla ed flasks with (2).		three times from ether; vacuum-sublimed twice;		
flasks	were suspended in an	open		purity not specified	
water bath and shaken gently from					
ments.	three weeks between : Samples of the repl		(2)	distilled and deioni:	zed.
ments. Samples of the replicate were extracted with cyclohexane.					
In all	cases, spectra taken	of			
second	extracts or of the a	queous			
⊥ayer a Comple+	fter extraction indi-	cated	L		
complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glass-		ESTIN	ATED ERROR:		
			• ± 0.5°C		
		soly	. see experimental va	alues	
			above		
Ware.		REFER	ENCES:		

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COMPONENTS:
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ORIGINAL MEASUREMENTS: (1) Acenaphthene; C₁₂H₁₀; [83-32-9] Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40, (2) Water; H₂O; [7732-18-5] 555-61. VARIABLES: PREPARED BY: One temperature: 25°C A. Maczynski

#### **EXPERIMENTAL VALUES:**

The solubility of acenaphthene in water at 25°C was reported to be 3.47 mg(l)/kg(2) and 2.2 x  $10^{-5}$  mol(l) dm⁻³(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are  $3.47 \times 10^{-4} \text{ g(1)}/100 \text{ g sln and } 4.05 \times 10^{-7}$ .

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with	<pre>(1) source not specified; analytical grade; used as received; no impurities by glc.</pre>		
hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<pre>(2) doubly distilled; free of trace organics.</pre>		
	ESTIMATED ERROR:		
	<pre>temp. ± 0.5°C soly. ± 0.06 mg(1)/kg(2) (from eight determinations)</pre>		
	REFERENCES:		

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of acenaphthene in wa to be 3.93 mg(1) dm ⁻³ sln and $x_1 = 4$	
The corresponding mass percent calcu is $3.93 \times 10^{-4}$ g(1)/100 g sln.	lated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was	<ul> <li>(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.</li> </ul>
decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs.	(2) doubly distilled.
the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American	
Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. $\pm$ 0.014 mg(1) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C.
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1980</u> , 14, 1227-9.
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of acenaphthene in wat mol/L sln. Assuming a solution densi mass per cent and mole fraction $(x_1)$ compiler, are 7.37 x $10^{-4}$ g(l)/100 g	ty of 1.00 kg/L the corresponding solubilities, calculated by the
	INFORMATION
METHOD/APPARATUS/PROCEDURE: Experiments were performed in sealed stainless steel centrifuge tubes. An excess of acenaphthene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at $25 \pm 0.2^{\circ}$ C with con- stant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to $25 \pm$ $0.3^{\circ}$ C, following which aliquots of the solution were removed for analy-	
the solution were removed for analy- sis by liquid scintillation counting. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.	ESTIMATED ERROR: Temperature: ±0.2°C Solubility: ±4.1% rel. (represent- ing one std. dev.) REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Rossi, S.S.; Thomas, W.H.
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1981</u> , 15, 715-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter
EXPERIMENTAL VALUES:	······································
The solubility of acenaphthene in dis be 2.42 µg/g, corresponding to a mole Corresponding mass per cent calculate g(l)/100 g sln.	fraction, $x_1$ , of 1.6 x 10 ⁻⁸ . The
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Flasks containing 500 mL of water and (1) were placed in a constant tempera ture (±0.1°C) gyrotary shaker (200 rpm) for at least 24 h. Following a 12 h stationary equilibration period, 100 mL of saturated solution was drained through a glass-wool plug int a separatory funnel. Acenaphthene Was isolated from solution by tripli- Cate extraction with 10 mL of hexane, which recovered over 99% of hydro- Carbon as determined in experiments With spiked solutions. Acenaphthene levels in concentrated extracts were determined on a Hewlett-Packard Model 5840A gas chromatograph using a WCOTSP-2100 glass column (30 m x 0.25 mm i.d.). Hydrocarbon concentrations in extracts were additionally deter- mined by ultraviolet spectrophoto- metry. Agreement was typically Within 2%. Further details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich; 99.9% purity; recryst. twice from dist. MeOH. (2) Doubly distilled in all-glass apparatus; free of trace organics. c ESTIMATED ERROR: Temperature: ±0.1°C Solubility: ±0.02 µg/g (std. dev. for 6 determinations) REFERENCES:</pre>

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Rossi, S.S.; Thomas, W.H.
(2) Seawater; natural	Environ. Sci. Technol. <u>1981</u> , 15, 715-6.
VARIABLES:	PREPARED BY:
Temperature: 15-25°C	W.Y. Shiu and D. Mackay
Salinity: 35 g/kg sln	
EXPERIMENTAL VALUES:	
Solubility of Acenar	
10 <u>t/°C μg(l)/g(2)</u> g(l	$\frac{5}{Mass } \frac{a}{a}$
15 0.214	2.14 2.56
20 0.55 25 1.84	5.5 6.6 18.4 22.0
^a Calculated by compilers	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solution was prepared by equilibrating seawater with an ex-	Acenaphthene: from Aldrich Chemical Co. of 99% purity and
cess of hydrocarbon for 24 hrs in a constant temperature gyrotary shaker	doubly distilled from distilled methanol,
followed by 12 hr stationary period.	n-Hexane: doubly distilled in glass,
A 100 mL-aliquot was extracted three times with n-hexane. The concen-	Seawater: collected off Scripps Pier
trated hexane extract was analyzed by a gas chromatograph equipped with	and was filtered twice through 0.22 µm membrane
a flame ionization detector to determine the hydrocarbon concentra-	and twice extracted with n-hexane then its salinity
tion.	adjusted to 35 %.
	Temp. $\pm 0.1^{\circ}$ K
	Soly. ±2%
	REFERENCES:

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COMPONENTS:	EVALUATOR:
<pre>(1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for biphenyl (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in biphenyl.

Bipheny	<u>yl (1) in Water (</u>	(2)
Reference	T/K	Method
Andrews and Keefer (ref 1)	298	spectrophotometric
Bohon and Claussen (ref 2)	274-316	spectrophotometric
Wauchope and Getzen (ref 4)	273-348	spectrophotometric
Ben-Naim <i>et al</i> . (ref 5)	283-323 ^a	spectrophotometric
Eganhouse and Calder (ref 6)	298	GLC
Mackay and Shiu (ref 7)	298	spectrofluorometric
Banerjee <i>et al</i> . (ref 8)	298	HPLC

TABLE 1: Quantitative Solubility Studies ofBiphenyl (1) in Water (2)

a Solubility on D₂O also reported.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition Bröllos *et al.* (ref 3) have studied the liquid-liquid phase equilibria in the biphenyl-water system at high temperatures and pressures, and Ben-Naim *et al.* (ref 5) have reported free energies of solution of biphenyl in  $D_2O$ .

All the available data on the solubility of biphenyl in water are summarized in Table 2 with the exception of the 298K data of Andrews and Keefer (ref 1) and Banerjee *et al.* (ref 8) which are substantially  $(>3\sigma_n)$  lower than all other values at this temperature (ref 2,4,6,7) and are therefore rejected. The data of Ben-Naim *et al.* (ref 5) expressed as free energies of solution have also been excluded.

In general the remaining data are in excellent agreement enabling values to be Recommended over a wide range of temperature. The data from Table 2 are also plotted in Figure 1.

COMPONENTS:	EVALUATOR:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

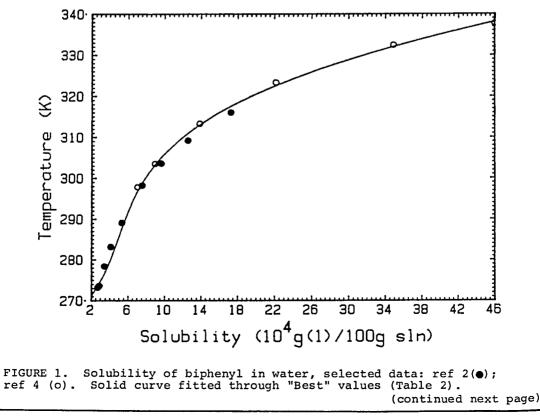
(continued) CRITICAL EVALUATION:

> TABLE 2: Recommended (R) and Tentative Values of the Solubility of Biphenyl (1) in Water (2)

T/K	Solubili	ty values	
	Reported values ^{$a$}	"Best" values	
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln	10 ⁷ x ₁
273	2.80* (ref 2), 2.64 (ref 4)	2.72 ± 0.08 (R)	3.2 (R)
283	4.06 (ref 2)	4.1	4.8
293	6.25* (ref 2)	6.3	7.4
298	7.48 (ref 2), 7.08 (ref 4), 7.45 (ref 6), 7.0 (ref 7)	7.2 ± 0.2 (R)	8.4 ( <i>R</i> )
303	9.4* (ref 2), 8.8* (ref 4)	9.1 ± 0.3 (R)	10.6 ( <i>R</i> )
313	15.1* (ref 2), 13.7* (ref 4)	$14.4 \pm 0.7 (R)$	16.8 (R)
323	22.0 (ref 4)	22	26
333	37.1* (ref 4)	37	43
1			

a Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the original data.
b Obtained by averaging where appropriate; σ_n has no statistical signifi-

cance.



COMPON	VENTS:	EVALUATOR:
(1)	Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	G.T. Hefter, School of Mathematical
	Water; H ₂ O; [7732-18-5]	and Physical Sciences, Murdoch University, Perth, W.A., Australia.
		June 1986.
CRITIC	CAL EVALUATION: (continued)	
REFE	RENCES	
1.	Andrews, L.J.; Keefer, R.M. J.	Am. Chem. Soc. <u>1949</u> , 71, 3644-7.
2.	Bohon, R.L.; Claussen, W.F. J.	Am. Chem. Soc. <u>1951</u> , 73, 1571-8.
з.	Bröllos, K.; Peter, K.; Schneider 1970, 74, 682-6.	c, G.M. Ber. Bunsenges. Phys. Chem.
4.	Wauchope, R.D.; Getzen, F.W. J.	Chem. Eng. Data <u>1972</u> , 17, 38-41.
5.	Ben-Naim, A.; Wilf, J.; Yaacobi,	M. J. Phys. Chem. <u>1973</u> , 77, 95-102.
6.	Eganhouse, R.P.; Calder, J.A. Ge 555-61.	eochim. Cosmochim. Acta <u>1976</u> , 40,
7.	Mackay, D.; Shiu, W.Y. J. Chem.	Eng. Data <u>1977</u> , 22, 399-402.
8.	Banerjee, S.; Yalkowski, S.H.; Va 1980, 14, 1227-9.	alvani, S.C. Environ. Sci. Technol.
ACUN		

ACKNOWLEDGEMENT

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The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of biphenyl in water a 0.000594 g(l)/l00 g sln. The corresponding mole fraction $x_1$ , c is 6.9 x $10^{-7}$ .	
15 6.9 X 10 .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C.	<pre>(1) Eastman Kodak Co. best grade; m.p. 70.0-70.5°C; used as received.</pre>
A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane	(2) not specified.
(10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase	
was measured against a hexane blank on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

<pre>(1) Bipheny1; C₁₂H₁₀; [92-52-4] (2) Water; H₂O; [7732-18-5] VARIABLES: Temperature: 0.4-42.8°C FYDERLYNNAL MALUEC.</pre> Bohon, R.L.; Claussen, W.F. J. Am. Chem. Soc. <u>1951</u> , 73, 1 G.T. Hefter	571-8.		
<pre>(2) Water; H₂O; [7732-18-5] J. Am. Chem. Soc. <u>1951</u>, 73, 1 VARIABLES: Temperature: 0.4-42.8°C G.T. Hefter</pre>	571-8.		
VARIABLES: Temperature: 0.4-42.8°C G.T. Hefter			
Temperature: 0.4-42.8°C G.T. Hefter			
Temperature: 0.4-42.8°C G.T. Hefter			
PVDEDTADURAL VALUES.			
EXPERIMENTAL VALUES: Solubility of biphenyl in water			
$t/^{\circ}$ C $10^{4}$ g(1)/100g sln ^a $10^{7}x_{1}$			
(compiler) (compiler)			
0.4 2.83 3.30	1		
2.4     2.97     3.47       5.2     3.38     3.94			
5.2         3.38         3.94           7.6         3.64         4.25			
10.0 4.06 4.74			
12.6 4.58 5.35			
14.9 5.11 5.96			
15.9 $5.27$ $6.1525.0 7.48^{b} 8.73^{b}$			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			
		33.3 11.0 12.8	
		34.9     11.9     13.9       36.0     12.5     14.6	
42.8 17.2 20.1			
^a Solubilities of (1) in (2) were reported as "optical density" (absormeasurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of $g(1)/L$ sln which was then converted to $g(1)/100g$ sln by assuming a solution density of 1.00 kg ^b Given in the paper as 7.48 x $10^{-3}g(1)/L$ sln.	ie ;'		
AUXILIARY INFORMATION			
METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS:			
A round-bottomed flask containing (1) Matheson Co., purified by			
about 4 mL of (1) and 400 mL of (2) recrystallization from abs Was evacuated, suspended in a methanol.	olute		
thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been	r, no		
tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of	1		
the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. ESTIMATED ERROR: Temp. ± 0.02°C Soly. ± 0.5% relative			
Absorbances were corrected for adsorption of (1) onto the walls			
of the cuvette. REFERENCES:			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.
VARIABLES:	PREPARED BY:
Temperature: 0-64.5°C	A. Maczynski
EXPERIMENTAL VALUES:	

	mg(1)/kg(		4	7
t/°C		smoothed with	$10^4$ g(l)/100 g sln	$10^{7}x_{1}$
]	experiment	(std dev)	(compiler)	(compiler)
0.0		2.64(0.07)	2.64	3.08
		· · · · ·	-	
24.6	7.13, 7.29, 7.35	6.96	6.96	8.13
25.0		7.08(0.09)	7.08	8.27
29.9	8.77, 8.64, 8.95	8.73	8.73	10.2
30.3	8.55, 8.54, 8.48	8.88	8.88	10.4
38.4	13.2, 13.3, 13.5	12.7	12.7	14.8
40.1	13.1, 13.4, 13.4	13.8	13.8	16.1
47.5	18.8, 19.0, 18.7	19.5	19.5	22.8
50.0		22.0(0.2)	22.0	25.7
50.1	20.6, 21.6, 21.8	22.1	22.1	25.8
50.2	20.7, 21.8	22.2	22.2	29.9
54.7	28.3, 28.8, 28.8	27.7	27.7	32.4
59.2	36.4, 36.3, 36.0	34.8	34.8	40.7
60.5	40.4	37.2	37.2	43.5
64.5	43.7, 44.7, 46.6	45.9	45.9	53.6

<pre>METHOD/APPARATUS/PROCEDURE: Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glass-</pre> SOURCE AND PURITY OF MATERIALS: SOURCE AND PURITY OF MATERIALS: SOURCE AND PURITY OF MATERIALS: SOURCE AND PURITY OF MATERIALS: (1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified. (2) distilled and deionized. ESTIMATED ERROR: temp. ± 0.5°C soly. see experimental values above	AUXILIARY	INFORMATION
<pre>in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by</pre> three times from ether; vacuum-sublimed twice; purity not specified. (2) distilled and deionized. (2) distilled and deionized. (2) distilled and deionized. (2) distilled and deionized. (2) distilled and deionized. (3) distilled and deionized. (4) distilled and deionized. (5) distilled and deionized. (2) distilled and deionized. (2) distilled and deionized. (3) distilled and deionized. (4) distilled and deionized. (5) distilled and deionized. (6) distilled and deionized. (7) distilled and deionized. (8) distilled and deionized. (8) distilled and deionized. (9) distilled and deionized. (9) distilled and deionized. (9) distilled and deionized. (1) distilled and deionized. (2) distilled and deionized. (2) distilled and deionized. (3) distilled and deionized. (4) distilled and deionized. (5) distilled and deionized. (6) distilled and deionized. (7) distilled and deionized. (8)		
Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by BESTIMATED ERROR: temp. ± 0.5°C soly. see experimental values above	in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated	three times from ether; vacuum-sublimed twice; purity not specified.
Cahn electrobalance, or by weighing soly. see experimental values		
	Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by	soly. see experimental values

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Ben-Naim, A.; Wilf, J.; Yaacobi, M.	
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1973</u> , 77, 95-102.	
VARIABLES:	PREPARED BY:	
Temperature: 10-50°C (282-323 K)	G.T. Hefter	
EXPERIMENTAL VALUES:		
The solubility of biphenyl in water	is expressed in terms of the standard	
free energy of solution, $\Delta \mu_{s}^{0}$ , determ		
	· *	
$\Delta \mu_{s}^{o} = \lim_{\rho \neq o \\ s \neq o \\ s$	[~] "( ^v s ^v s ^v eq ⁻	
where $\left(a^{l}/a^{q}\right)$ is the Ostwald absor	ration coofficient and a ^l and a ^g are	
where $(\rho_s^{\ell} / \rho_s^{q})_{eq}$ is the Ostwald absorption coefficient and $\rho_s^{\ell}$ and $\rho_s^{q}$ are respectively the molar concentrations of the solute s in the liquid and		
the gas phase at equilibrium.		
For the temperature range studied, A	$^{\mu}s$ was fitted to a second degree	
polynomial of the form:		

 $\Delta \mu_{\rm S}^{\rm o} = -14740.4 + 52.057 t - 0.04126 t^2$ 

where t is in °C (10 < t < 50°C) and  $\Delta \mu_{s}^{o}$  is in cal/mol (1 cal = 4.184 J).

Values of the Ostwald absorption coefficient are also reported.

### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubilities were determined spectro- scopically. Saturated solutions were prepared in two ways: (a) direct mixing of benzene and water for ca. 48 h, (b) dissolution of benzene through the vapor phase. Absorbances of the solutions and their vapors were measured directly at $\lambda_{max}$ with a Model 450 Perkin-Elmer spectro- photometer with a thermostatted cell holder. Establishment of equilibrium was checked by use of a special three	<ol> <li>Fluka; puriss, 99.94%, used as received.</li> <li>Distilled water, further distilled from alk. KMnO₄ and acid K₂Cr₂O₇; κ, 0.8 x 10⁻⁶S cm⁻¹.</li> </ol>
Compartment cell, details of which	ESTIMATED ERROR:
are given in the paper.	Temperature: ±0.05°C Solubility: std. dev. in Δμ ⁰ , 22.794 cal/mol.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Eganhouse, R.P.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	······································
The solubility of biphenyl in water a to be 3.47 mg(l)/kg(2) and 4.8 x $10^{-5}$	$mol(1) dm^{-3}(2).$
The corresponding mass percent and mo by the compiler are 7.45 x $10^{-4}$ g(1)/	ble fraction, $x_1$ , calculated
by the complier are 7.45 x 10 $g(1)/$	$100 \text{ g sin and } 8.70 \text{ x } 10^{-1}$ .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) source not specified; analytical grade; used as received; no impurities by glc.</li> <li>(2) doubly distilled; free of trace organics.</li> </ul>
	ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.06 mg(1)/kg(2) (from eight determinations)
	REFERENCES :

349
ORIGINAL MEASUREMENTS:
Mackay, D.; Shiu, W.Y.
J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
PREPARED BY:
M.C. Haulait-Pirson
<b>_</b>
at 25°C was reported .15 x 10 ⁻⁷ . Alated by the compiler
INFORMATION
<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled.  ESTIMATED ERROR: soly. ± 0.06 mg(1) dm⁻³ sln (maximum deviation from several determinations.)  REFERENCES: </pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Water; H ₂ O; [7732-18-5]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Environ. Sci. Technol. <u>1980</u> , 14, 1227-9.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	G.T. Hefter	
EXPERIMENTAL VALUES:		

The solubility of biphenyl in water was reported to be  $3.91 \times 10^{-5} \text{ mol/L}$  sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction,  $x_1$ , solubilities, calculated by the compiler, are  $6.03 \times 10^{-4} \text{ g(1)/100 g sln}$  and  $7.05 \times 10^{-7}$ .

AUXILIARY	INFORMATION
	THE OLG TIL TON

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Experiments were performed in sealed stainless steel centrifuge tubes. An excess of biphenyl was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at $25 \pm 0.2^{\circ}$ C with con- stant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to $25 \pm$	<ol> <li>Aldrich; purity not specified.</li> <li>Distilled.</li> </ol>		
0.3°C, following which aliquots of the solution were removed for analy-	TOMTICIANTE TEROP		
	ESTIMATED ERROR:		
chromacography using a waters Moutur	Temperature: ±0.2°C		
	Solubility: ±6.0% rel. (represent- ing one std. dev.)		
	REFERENCES:		

	35
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Ben-Naim, A.; Wilf, J.; Yaacobi, M.
<pre>(2) Deuterium oxide (Heavy water); D₂O; [7789-20-0]</pre>	J. Phys. Chem. <u>1973</u> , 77, 95-102.
VARIABLES:	PREPARED BY:
Temperature: 10-50°C	G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of biphenyl in heavy w standard free energy of solution, $\Delta \mu_{s}^{0}$	
$\Delta \mu_{g}^{\circ} = \lim_{\substack{\rho_{g}^{\rightarrow} \circ}} \left[-RT \ln \left(\rho_{g}^{\ell} / \rho_{g}^{g}\right)\right]$	ed]
where $(\rho_s^{\ell}/\rho_s^{g})_{eq}$ is the Ostwald absorp respectively the molar concentrations the gas phase at equilibrium.	tion coefficient and $\rho_{S}^{l}$ and $\rho_{S}^{g}$ are of the solute s in the liquid and
For the temperature range studied, $\Delta \mu$ polynomial of the form:	$_{\rm s}^{\circ}$ was fitted to a second degree
$\Delta \mu_{s}^{0} = -12827.6 + 39.059$	$t - 0.01945 t^2$
where t is in °C (10 < $t$ < 50°C) and	$\Delta \mu_{\rm S}^{\rm o}$ is in cal/mol (1 cal = 4.184 J).
Values of the Ostwald absorption coef	ficient are also reported.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubilities were determined spectro- scopically. Saturated solutions were prepared in two ways: (a) direct mixing of benzene and water for <i>ca</i> . 48 h, (b) dissolution of benzene through the vapor phase. Absorbances of the solutions and their vapors	received. (2) Fluka, 99.75%, used as received
were measured directly at $\lambda_{max}$ with a Model 450 Perkin-Elmer spectrophoto- meter with a thermostatted cell holder. Establishment of equilibrium was checked by use of a special three	
compartment cell, details of which ESTIMATED ERROR:	
are given in the paper.	Temperature: $\pm 0.05^{\circ}$ C Solubility: std. dev. in $\Delta \mu_{S}^{\circ}$ ,
	270.15 cal/mol.

COMPONENTS: (1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) Seawater D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of biphenyl (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10 ⁴ g(l)/100 g sln
Paul (ref l)	uv spectral	13-64	6.08 - 3.45
Eganhouse and Calder (ref 2)	GLC	35	4.76

The reported data are all from different salinities which precludes direct comparison. Since the data appear consistent with each other and with the recommended value for the solubility of biphenyl in pure water, the data of Paul and of Eganhouse and Calder are adopted as tentative.

	SOLUBILITY OF	BIPHENYL (1) IN	SEAWATER	(2)
		TENTATIVE VALUE		
т/к		g salts/kg sln		10 ⁴ g(l)/100 g sln
—				<u> </u>
298		35		4.76

#### REFERENCES

- 1. Paul, M.A. J. Amer. Chem. Soc. 1952, 74, 5274-7.
- 2. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40, 555-61.

COMPONENTS:		
	ORIGINAL MEASUREMENTS:	
<ol> <li>Biphenyl; C₁₂H₁₀; [92-52-4]</li> <li>Sodium chloride; NaCl; [7732-14-5]</li> <li>Water; H₂O; [7647-18-5]</li> </ol>	Paul, M.A. J. Am. Chem. Soc. <u>1952</u> , 74, 5274-7.	
VARIABLES :	PREPARED BY:	
One temperature: 25°C		
Salinity: 13-64 g(3)/kg sln	M. Kleinschmidt and W. Shiu	
EXPERIMENTAL VALUES:		
Solubility of Biphenyl an	d Aqueous Sodium Chloride	
mol(2)/L g(2)/kg sln [*] 10 ⁵ m	$101(1)/L$ $10^4$ Mass $\frac{10^7 x_1}{1}$	
0.687         39.05         3.           0.818         46.28         2.           0.916         51.62         2.           1.145         63.97         2.	40         3.54         4.32           34         3.45         4.21	
AUXILIARY	INFORMATION	
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:	

COMPONENTS: ORIGINAL MEASUREMENTS: Eganhouse, R.P.; Calder, J.A. (1) Biphenyl; C₁₂H₁₀; [92-52-4] Geochim. Cosmochim. Acta 1976, 40, (2) Artificial seawater (ref 1) 555-61. VARIABLES: PREPARED BY: One temperature: 25.0°C M. Kleinschmidt and W. Shiu Salinity: 35 g/kg sln EXPERIMENTAL VALUES: The solubility of biphenyl in seawater is reported to be 4.76 mg/kg. The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compilers are 4.76 x  $10^{-4}$  g(1)/100 g sln and 5.70 x  $10^{-7}$ . Graphical results for other salinities are also reported. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Equilibrium flask: 1-dm³ Erlen-(1) analytical grade salts for meyer flask with ground glass artificial seawater solution, stopper and sidearm tap at base plugged with glass wool. The reagent grade. mixtures were agitated 12+ hr at water: doubly distilled 215 rpm on a New Brunswick gyrotary shaker; a 24 hr stationary equilibrium period followed. Hydrocarbons were extracted with doubly-distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal **ESTIMATED ERROR:** standard. temperature: ± 0.5°C Analysis: gas chromatography ± 0.293 (95% confidence soly: interval). **REFERENCES:** Lyman, J.; Fleming, R.H.; J. Mar. Res. <u>1940</u>, 3, 135.

	355
COMPONENTS :	ORIGINAL MEASUREMENTS:
<ol> <li>1,3-Dimethylnaphthalene; C₁₂H₁₂;</li> </ol>	Mackay, D.; Shiu, W.Y.
[575-41-7]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1,3-dimethylnaphth	alene in water at 25°C was reported
to be 8.0 mg(1) dm ⁻³ sln and $x_1 = 9.3$	$2 \times 10^{-7}$ .
The corresponding mass percent calcu	lated by the compiler
is 8.0 x $10^{-4}$ g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL	<ol> <li>Aldrich Chemicals, Eastman Kodak, or K and K Laboratories,</li> </ol>
flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	commercial highest grade; used as received.
Then the saturated solution was decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	
funnel. After shaking for 2 hrs.	
the cyclohexane extract was removed for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. ± 0.5 mg(1) dm ⁻³ sln (maximum deviation from several
	determinations).
	REFERENCES :
1	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dimethylnaphthalene; C ₁₂ H ₁₂ ;	
[571-58-4]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1,4-dimethylnaphth	
to be 11.4 mg(1) dm ⁻³ sln and $x_1 = 1$	$.31 \times 10^{-6}$ .
The corresponding mass percent calcu	lated by the compiler
is 0.00114 g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2)	(1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently	Kodak, or K and K Laboratories, commercial highest grade;
settled at 25°C for at least 48 hrs.	used as received.
Then the saturated solution was decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	]
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. $\pm$ 0.1 mg(1) dm ⁻³ sln
	(maximum deviation from several determinations).
	REFERENCES :
	S. EALITOLD,
	l

COMPONENTS: (1) 1,5-Dimethylnaphthalene; C ₁₂ H ₁₂ ; [571-61-9] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences,
-	Warszawa, Poland.
	June 1986.
CRITICAL EVALUATION:	

Quantitative solubility data for 1,5-dimethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1,5-dimethylnaphthalene.

## TABLE 1: Quantitative Solubility Studies of1,5-Dimethylnaphthalene (1) in Water (2)

Reference	T/K	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The two values available (Table 1), obtained by different methods, are in reasonable agreement and their mean can be considered as a Tentative value (Table 2).

# TABLE 2: Tentative Value of the Solubility of 1,5-Dimethylnaphthalene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value $(\pm \sigma_n)^{\alpha}$	
	10 ⁴ g(1)/100g sln	$10^4$ g(1)/100g sln $10^7 x_1$	
298	2.74 (ref 1), 3.38 (ref 2)	3.1 ± 0.3 3.6	

a Obtained by averaging;  $\boldsymbol{\sigma}_n$  has no statistical significance.

### REFERENCES

- Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.
- 2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

	ODICINAL MEASUREMENTS
COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>(1) 1,5-Dimethylnaphthalene; C₁₂H₁₂; [571-61-9]</li> <li>(2) Water; H₂O; [7732-18-5]</li> </ol>	Eganhouse, R.P.; Calder, J.A.
	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1,5-dimethylnaphthat reported to be 2.74 mg(1)/kg(2) and 1	
The corresponding mass percent and motor by the compiler are 2.74 x $10^{-4}$ g(1)/	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with	<pre>(1) source not specified; analytical grade; used as received; no impurities by glc.</pre>
hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<pre>(2) doubly distilled; free of trace organics.</pre>
-	ESTIMATED ERROR:
	<pre>temp. ± 0.5°C soly. ± 0.1 mg(1)/kg(2) (from eight determinations)</pre>
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
<ol> <li>1,5-Dimethylnaphthalene;</li> </ol>	Mackay, D.; Shiu, W.Y.
C ₁₂ H ₁₂ ; [571-61-9]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
(2) Water; H ₂ O; [7732-18-5]	333 4021
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1,5-dimethylnaphth to be 3.38 mg(1) dm ⁻³ sln and $x_1 = 3$	
The corresponding mass percent calcu is 3.38 x $10^{-4}$ g(1)/100 g sln.	lated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman	(2) doubly distilled.
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. ± 0.04 mg(l) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES:

COMPONENTS :	EVALUATOR:
<ul> <li>(1) 2,3-Dimethylnaphthalene; C₁₂H₁₂; [581-40-8]</li> <li>(2) Water; H₂O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.
1	
	June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for 2,3-dimethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 2,3-dimethylnaphthalene.

### TABLE 1:Quantitative Solubility Studies of2,3-Dimethylnaphthalene(1)in Water(2)

Reference	T/K	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometri

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The two values available (Table 1), obtained by different methods, are in reasonable agreement and their mean can be considered as a Tentative value (Table 2).

TABLE 2: Tentative Value of the Solubility of 2,3-Dimethylnaphthalene (1) in Water (2)

T/K	Solubility	Solubility values	
	Reported values	"Best" value	
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln	10 ⁷ x1
298	1.99 (ref 1), 3.0 (ref 2)	2.5 ± 0.5	2.9
a Ob	tained by averaging; $\sigma_n$ has no statistica	al significance.	<u> </u>
REFE	RENCES		
1.	Eganhouse, R.P.; Calder, J.A. <i>Geochim</i> . 555-61.	Cosmochim. Acta 197	<u>6</u> , 40,
2.	Mackay, D.; Shiu, W.Y. J. Chem. Eng. Do	ata <u>1977</u> , 22, 399-40	2.

p	
COMPONENTS :	ORIGINAL MEASUREMENTS:
<ul> <li>(1) 2,3-Dimethylnaphthalene; C₁₂H₁₂; [581-40-8]</li> <li>(2) Water; H₂O; [7732-18-5]</li> </ul>	Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 2,3-dimethylnaphtha reported to be 1.99 mg(1)/kg(2) and 1	$.3 \times 10^{-5} mol(1) dm^{-3}(2)$ .
The corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are 1.99 x $10^{-4}$ g(1)/100 g sln and 2.29 x $10^{-7}$ .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<ol> <li>source not specified; analytical grade; used as received; no impurities by glc.</li> <li>doubly distilled; free of trace organics.</li> </ol>
	ESTIMATED ERROR:
	<pre>temp. ± 0.5°C soly. ± 0.02 mg(1)/kg(2) (from eight determinations)</pre>
	REFERENCES :

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ORIGINAL MEASUREMENTS:
COMPONENTS:

 2,3-Dimethylnaphthalene; C<sub>12</sub>H<sub>12</sub>;

 Mackay, D.; Shiu, W.Y.
 [581-40-8]
 J. Chem. Eng. Data 1977, 22,
 399-402.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
VARIABLES:
 PREPARED BY:
 One temperature: 25°C
 M.C. Haulait-Pirson
EXPERIMENTAL VALUES:
 The solubility of 2,3-dimethylnaphthalene in water at 25°C was reported
 to be 3.0 mg(1) dm<sup>-3</sup> sln and x_1 = 3.47 \times 10^{-7}.
 The corresponding mass percent calculated by the compiler
 is 3.0 \times 10^{-4} g(1)/100 g sln.
 AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:
 SOURCE AND PURITY OF MATERIALS:
 A saturated solution of (1) in (2)
 (1) Aldrich Chemicals, Eastman
 was vigorously stirred in a 250 mL
 Kodak, or K and K Laboratories,
 flask for 24 hrs. and subsequently
 commercial highest grade;
 settled at 25°C for at least 48 hrs.
 used as received.
 Then the saturated solution was
 decanted and filtered and 50-100 mL
 (2) doubly distilled.
 extracted with approximately 5 mL
 of cyclohexane in a separatory funnel. After shaking for 2 hrs.
 the cyclohexane extract was removed
 for analysis. An Aminco-Browman
 spectrophotofluorometer (American
 Instruments Ltd.) was used for
 ESTIMATED ERROR:
 analysis. Many details are given
 soly. \pm 0.01 mg(1) dm<sup>-3</sup> sln
 in the paper.
 (maximum deviation from several
 determinations).
 REFERENCES:
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COMPONENTS :		
	EVALUATOR: G.T. Hefter, S	chool of Mathematical ciences, Murdoch
<pre>(1) 2,6-Dimethylnaphthalene; C₁₂H₁₂; [581-42-0]</pre>	University, Pe A. Maczynski,	rth, W.A., Australia. Institute of Physical
(2) Water; H ₂ O; [7732-18-5]	Warszawa, Pola	ish Academy of Sciences nd.
	June 1986.	
CRITICAL EVALUATION:		
Quantitative solubility data for 2,6-0	dimethylnaphtha	lene (1) in water (2)
have been reported in the publication		
been reported on the solubility of war	ter in 2,6-dime	thylnaphthalene.
TABLE 1: Quantitative2,6-Dimethylnaphtha		
Reference	Т/К	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)		spectrofluorometric
	an be considere	d as a Tentative value
(Table 2). TABLE 2: Tentative Va	alue of the Sol	ubility of
(Table 2).	alue of the Sol	ubility of
(Table 2). <u>TABLE 2: Tentative Va</u> <u>2,6-Dimethylnaphtha</u>	alue of the Sol alene (1) in Wa ubility values	ubility of ter (2)
(Table 2). <u>TABLE 2: Tentative Va</u> <u>2,6-Dimethylnaphtha</u> <i>T/K</i> Solu Reported values	alue of the Sol alene (1) in Wa ubility values	ubility of ter (2) "Best" value (± σ _n ) ^α
(Table 2). <u>TABLE 2: Tentative Va</u> <u>2,6-Dimethylnaphtha</u> T/K Solu	alue of the Sol alene (1) in Wa ubility values	ubility of ter (2)
(Table 2). <u>TABLE 2: Tentative Va</u> <u>2,6-Dimethylnaphtha</u> <i>T/K</i> Solu Reported values	alue of the Solatene (1) in War ubility values 10 ⁴ g(1)	ubility of ter (2) "Best" value (± σ _n ) ^α
(Table 2). <u>TABLE 2: Tentative Va</u> <u>2,6-Dimethylnaphtha</u> <i>T/K</i> Solu Reported values 10 ⁴ g(1)/100g sln	alue of the Sol alene (1) in Wa ubility values 10 ⁴ g(1) 1.	ubility of ter (2) "Best" value $(\pm \sigma_n)^a$ )/loog sln $10^7 x_1$ 7 ± 0.4 2.0
<pre>(Table 2). <u>TABLE 2: Tentative Va</u> <u>2,6-Dimethylnaphtha</u> T/K Solu Reported values 10⁴g(1)/100g sln 298 1.30 (ref 1), 2.0 (ref 2) a Obtained by averaging; σ_n has no state a Obtained by averaging a Obtained by averaging; σ_n has no state a Obtained by averaging a Obtained</pre>	alue of the Sol alene (1) in Wa ubility values 10 ⁴ g(1) 1.	ubility of ter (2) "Best" value $(\pm \sigma_n)^a$ )/loog sln $10^7 x_1$ 7 ± 0.4 2.0
(Table 2). <u>TABLE 2: Tentative Va</u> <u>2,6-Dimethylnaphtha</u> T/K Solu Reported values 10 ⁴ g(1)/100g sln 298 1.30 (ref 1), 2.0 (ref 2) a Obtained by averaging; $\sigma_n$ has no sta REFERENCES	alue of the Soli alene (1) in War ubility values 10 ⁴ g(1) 1. atistical signi	ubility of ter (2) "Best" value $(\pm \sigma_n)^a$ )/100g sln $10^7 x_1$ 7 ± 0.4 2.0 ficance.
<pre>(Table 2). <u>TABLE 2: Tentative Va</u> <u>2,6-Dimethylnaphtha</u> T/K Solu Reported values 10⁴g(1)/100g sln 298 1.30 (ref 1), 2.0 (ref 2) a Obtained by averaging; σ_n has no state a Obtained by averaging a Obtained by averaging; σ_n has no state a Obtained by averaging a Obtained</pre>	alue of the Soli alene (1) in War ubility values 10 ⁴ g(1) 1. atistical signi	ubility of ter (2) "Best" value $(\pm \sigma_n)^a$ )/100g sln $10^7 x_1$ 7 ± 0.4 2.0 ficance.
<pre>(Table 2). <u>TABLE 2: Tentative Vanta Vanta 2,6-Dimethylnaphtha</u> T/K Solu Reported values 10⁴g(1)/100g sln 298 1.30 (ref 1), 2.0 (ref 2) a Obtained by averaging; o_n has no state REFERENCES 1. Eganhouse, R.P.; Calder, J.A. Gauge 2010 1. Eganhouse, R.P.; Calder, J.A. Gauge 2010 Control of the second state Control of</pre>	alue of the Soliaiene (1) in War ability values 10 ⁴ g(1) 1. atistical signit	ubility of $\frac{\text{ter (2)}}{\text{"Best" value } (\pm \sigma_n)^a}$ )/loog sln $10^7 x_1$ 7 ± 0.4 2.0 ficance. <i>im. Acta</i> <u>1976</u> , 40,
(Table 2). $\frac{\text{TABLE 2: Tentative Va}}{2,6-\text{Dimethylnaphtha}}$ T/K Solu Reported values $10^4 \text{g}(1)/100 \text{g sln}$ 298 1.30 (ref 1), 2.0 (ref 2) a Obtained by averaging; $\sigma_n$ has no state REFERENCES 1. Eganhouse, R.P.; Calder, J.A. Gauge 10, 10, 10, 10, 10, 10, 10, 10, 10, 10,	alue of the Soliaiene (1) in War ability values 10 ⁴ g(1) 1. atistical signit	ubility of $\frac{\text{ter (2)}}{\text{"Best" value } (\pm \sigma_n)^a}$ )/loog sln $10^7 x_1$ 7 ± 0.4 2.0 ficance. <i>im. Acta</i> <u>1976</u> , 40,
(Table 2). $\frac{\text{TABLE 2: Tentative Va}}{2,6-\text{Dimethylnaphtha}}$ $T/K \qquad \text{Solu}$ Reported values $10^4 \text{g(1)}/100 \text{g sln}$ 298 1.30 (ref 1), 2.0 (ref 2) $a \text{ Obtained by averaging; } \sigma_n \text{ has no sta}$ REFERENCES 1. Eganhouse, R.P.; Calder, J.A. Gauge 555-61.	alue of the Soliaiene (1) in War ability values 10 ⁴ g(1) 1. atistical signit	ubility of $\frac{\text{ter (2)}}{\text{"Best" value } (\pm \sigma_n)^a}$ )/loog sln $10^7 x_1$ 7 ± 0.4 2.0 ficance. <i>im. Acta</i> <u>1976</u> , 40,
(Table 2). $\frac{\text{TABLE 2: Tentative Va}}{2,6-\text{Dimethylnaphtha}}$ $T/K \qquad \text{Solu}$ Reported values $10^4 \text{g(1)}/100 \text{g sln}$ 298 1.30 (ref 1), 2.0 (ref 2) $a \text{ Obtained by averaging; } \sigma_n \text{ has no sta}$ REFERENCES 1. Eganhouse, R.P.; Calder, J.A. Gauge 555-61.	alue of the Soliaiene (1) in War ability values 10 ⁴ g(1) 1. atistical signit	ubility of $\frac{\text{ter (2)}}{\text{"Best" value } (\pm \sigma_n)^a}$ )/loog sln $10^7 x_1$ 7 ± 0.4 2.0 ficance. <i>im. Acta</i> <u>1976</u> , 40,
(Table 2). $\frac{\text{TABLE 2: Tentative Va}}{2,6-\text{Dimethylnaphtha}}$ $T/K \qquad \text{Solu}$ Reported values $10^4 \text{g(1)}/100 \text{g sln}$ 298 1.30 (ref 1), 2.0 (ref 2) $a \text{ Obtained by averaging; } \sigma_n \text{ has no sta}$ REFERENCES 1. Eganhouse, R.P.; Calder, J.A. Gauge 555-61.	alue of the Soliaiene (1) in War ability values 10 ⁴ g(1) 1. atistical signit	ubility of ter (2) "Best" value $(\pm \sigma_n)^a$ )/loog sln $10^7 x_1$ 7 ± 0.4 2.0 ficance. im. Acta <u>1976</u> , 40,

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) 2,6-Dimethylnaphthalene; C₁₂H₁₂; [581-42-0]</li> <li>(2) Water; H₂O; [7732-18-5]</li> </ul>	Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	La
The solubility of 2,6-dimethylnaphtha reported to be 1.30 mg(l)/kg(2) and 8 The corresponding mass percent and mo by the compiler are 1.30 x 10 ⁻⁴ g(l)/	$x_{3} \times 10^{-6} \text{ mol}(1) \text{ dm}^{-3}(2).$
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	glc. (2) doubly distilled; free of trace organics.
	ESTIMATED ERROR:
	temp. ± 0.5°C soly. ± 0.04 mg(1)/kg(2)

soly. ± 0.04 mg(l)/kg(2) (from eight determinations)

**REFERENCES:** 

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2,6-Dimethylnaphthalene;	Mackay, D.; Shiu, W.Y.
C _{12^H12} ; [581-42-0]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2,6-dimethylnaphthat to be 2.0 mg(1) dm ⁻³ sln and $x_1 = 2.3$	$33 \times 10^{-7}$ .
The corresponding mass percent calcul is 2.0 x $10^{-4}$ g(1)/100 g sln.	lated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman	(2) doubly distilled.
spectrophotofluorometer (American	
Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. $\pm$ 0.02 mg(l) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES:

COMPONENTS :	EVALUATOR:
<pre>(1) 1-Ethylnaphthalene; C₁₂H₁₂; [1127-76-0] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.
1	April 1986.

#### CRITICAL EVALUATION:

Quantitative solubility data for 1-ethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1-ethylnaphthalene.

### TABLE 1: Quantitative Solubility Studies of1-Ethylnaphthalene (1) in Water (2)

Reference	T/K	Method
Mackay and Shiu (ref 1)	298	spectrofluorometric
Schwarz and Wasik (ref 2)	282-305	spectrophotometric
Schwarz (ref 3)	284-298	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The data available (Table 1) are summarized in Table 2 and plotted in Figure 1. For the purpose of this Evaluation the values of Schwarz (ref 3) are not considered as independent determinations. Nevertheless, the excellent agreement between the data of Schwarz and Wasik (ref 2,3) and Mackay and Shiu (ref 1) at 298K suggests the values of Schwarz and Wasik at other temperatures can be considered as Tentative.

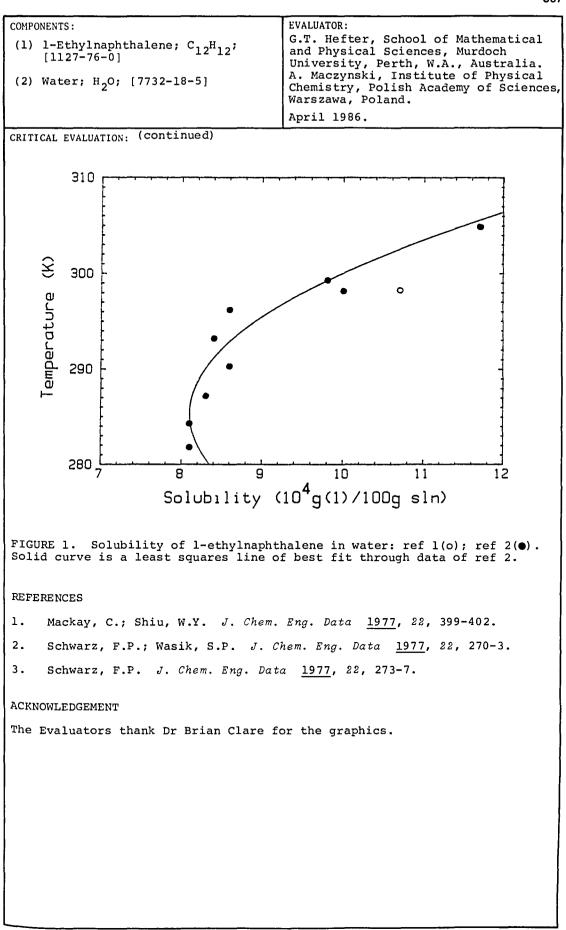
 TABLE 2: Recommended (R) and Tentative Solubility Values of

 1-Ethylnaphthalene (1) in Water (2)

T/K Solubi		ty values	
	Reported values ^a	"Best" valu	
	10 ⁴ g(1)/100g sln	10 ⁴ g(l)/100g sln	10 ⁷ x1
283	8.1 (ref 2), 8.1* (ref 3)	8.1	9.4
293	10.0 (ref 2), 8.5* (ref 3)	8.5	9.8
298	10.7 (ref 1), 10.0 (ref 2), 9.5* (ref 3)	10.1 ± 0.5 (R)	11.6 ( <i>R</i> )
303	11.0* (ref 3)	11	13

a Values marked with an asterisk (*) were obtained by the Evaluators by graphical interpolation of the authors' original data.

b Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance.



COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>(1) 1-Ethylnaphthalene; C₁₂H₁₂;</li> </ol>	Mackay, D.; Shiu, W.Y.
[1127-76-0]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
	A.C. hadiait-filboh
EXPERIMENTAL VALUES:	
	·
The solubility of 1-ethylnaphthalene	in water at 25°C was reported
to be 10.7 mg(1) dm ⁻³ sln and $x_1 = 1$ .	$24 \times 10^{-6}$ .
mbe serves ains mess noncent select	stad by the compiler
The corresponding mass percent calcul is 0.00107 g(1)/100 g sln.	ated by the compiler
15 0.00107 g(1)/100 g 51n.	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL	<ul> <li>(1) Aldrich Chemicals, Eastman</li> <li>Kodak, or K and K Laboratories,</li> </ul>
flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	commercial highest grade; used as received.
Then the saturated solution was	
decanted and filtered and 50-100 mL extracted with approximately 5 mL	(2) doubly distilled.
of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. $\pm$ 0.3 mg(1) dm ⁻³ sln
in the paper.	(maximum deviation from several determinations).
	REFERENCES :
1	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) 1-Ethylnaphthalene; C₁₂^H12; [1127-76-0]</pre>	Schwarz, F.P.	
	J. Chem. Eng. Data 1	977, 22, 273-7.
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
Temperature: 8.6-31.7°C	A. Maczynski	
EXPERIMENTAL VALUES:	I	
Solubility of 1-ethyln	aphthalene in water	
5 _1		7
t/°C 10 ⁵ mol(1) L ⁻¹	10 ⁴ g(1)/100 g sln (compiler)	$10^{7}x_{1}$ (compiler)
8.6 5.2 ± 0.3	8.1	9.4
11.1 5.2 ± 0.2	8.1	9.4
14.0 5.3 ± 0.1	8.3	9.5
17.1 5.5 ± 0.1	8.6	9.9
20.0 5.4 ± 0.1	8.4	9.7
23.0 5.5 ± 0.1	8.6	9.9
25.0 6.4 ± 0.1	10.0	11.5
26.1 6.3 ± 0.1	9.8	11.3
31.7 7.5 ± 0.2	11.7	13.5
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATER	IALS:
Two methods were used.	(1) source not specif:	
At 25°C the solubility of (1) in (2)	than 99.9 mole%, h used as received.	by glc;
was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.	(2) distilled over KMr and passed through column.	
The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.	ESTIMATED ERROR: temp. ± 0.1°C soly. see above	<u></u>
	REFERENCES :	<u> </u>

COMPONENTS:		ORIGINAL MEASUREMENTS:		
			a 5	
<pre>(1) 1-Ethylnaphthalene; C₁₂H₁₂; [1127-76-0] (2) Water; H₂O; [7732-18-5]</pre>		Schwarz, F.P.; Wasik,		
		J. Chem. Eng. Data <u>19</u>	<u>77</u> , 22, 270-3.	
(2) Mater	, ¹ ₂ 0, [,,,,,, 10, 5]			
VARIABLES: Temperature: 10-25°C		PREPARED BY:	PREPARED BY: A. Maczynski	
		A. Maczynski		
EXPERIMENTAL	VALUES:	· · <b>I</b> · · · · · · · · · · · · · · · · · · ·		
	Solubility of 1-ethy:	lnaphthalene in water		
t/°C	10 ⁵ mol(1) L ⁻¹	10 ⁴ g(1)/100 g sln (compiler)	$10^7 x_1$ (compiler)	
10	5.2 ± 0.2	8.1	9.4	
14	5.2 ± 0.1	8.1	9.4	
20	6.4 ± 0.1	10.0	11.5	
25	6.4 ± 0.1	10.0	11.5	
	AUXILIA	ARY INFORMATION		
ME THOD / AP P A	AUXILIA RATUS/PROCEDURE:	ARY INFORMATION SOURCE AND PURITY OF MATERI	ALS:	
The solut determine Since the (2) are extincted the absor- performed the satu:		SOURCE AND PURITY OF MATERI (1) Chemical Samples ( Columbus, Ohio; be 99.9 mole%.	Co., etter than nO4 and passed	
The solut determine Since the (2) are the extinction the absor- performed the satur	RATUS/PROCEDURE: bility of (1) in (2) was ed from its absorbance. e concentration of (1) in too low to determine its on coefficient accurately, rption measurements were d on measured volumes of rated solutions diluted	<ul> <li>SOURCE AND PURITY OF MATERI</li> <li>(1) Chemical Samples ( Columbus, Ohio; ba 99.9 mole%.</li> <li>(2) distilled from KMn through a Sephades</li> <li>ESTIMATED ERROR:</li> </ul>	Co., etter than nO4 and passed	
The solut determine Since the (2) are the extinction the absor- performed the satur	RATUS/PROCEDURE: bility of (1) in (2) was ed from its absorbance. e concentration of (1) in too low to determine its on coefficient accurately, rption measurements were d on measured volumes of rated solutions diluted	<ul> <li>SOURCE AND PURITY OF MATERI</li> <li>(1) Chemical Samples ( Columbus, Ohio; ba 99.9 mole%.</li> <li>(2) distilled from KMn through a Sephades</li> </ul>	Co., etter than nO4 and passed	
The solut determine Since the (2) are the extinction the absor- performed the satur	RATUS/PROCEDURE: bility of (1) in (2) was ed from its absorbance. e concentration of (1) in too low to determine its on coefficient accurately, rption measurements were d on measured volumes of rated solutions diluted	<pre>SOURCE AND PURITY OF MATERI (1) Chemical Samples (     Columbus, Ohio; be     99.9 mole%. (2) distilled from KMm     through a Sephade:     ESTIMATED ERROR:     temp. ± 0.1°C</pre>	Co., etter than nO4 and passed	
The solut determine Since the (2) are the extinction the absor- performed the satur	RATUS/PROCEDURE: bility of (1) in (2) was ed from its absorbance. e concentration of (1) in too low to determine its on coefficient accurately, rption measurements were d on measured volumes of rated solutions diluted	<ul> <li>SOURCE AND PURITY OF MATERI</li> <li>(1) Chemical Samples ( Columbus, Ohio; be 99.9 mole%.</li> <li>(2) distilled from KMn through a Sephades</li> <li>ESTIMATED ERROR: temp. ± 0.1°C soly. see above</li> </ul>	Co., etter than nO4 and passed	
The solut determine Since the (2) are the extinction the absor- performed the satur	RATUS/PROCEDURE: bility of (1) in (2) was ed from its absorbance. e concentration of (1) in too low to determine its on coefficient accurately, rption measurements were d on measured volumes of rated solutions diluted	<ul> <li>SOURCE AND PURITY OF MATERI</li> <li>(1) Chemical Samples ( Columbus, Ohio; be 99.9 mole%.</li> <li>(2) distilled from KMn through a Sephades</li> <li>ESTIMATED ERROR: temp. ± 0.1°C soly. see above</li> </ul>	Co., etter than nO ₄ and passed	

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Ethylnaphthalene; C₁₂H₁₂; [1127-76-0]</pre>	Schwarz, F.P.
<pre>(2) Sodium chloride; NaCl; [7647-14-5]</pre>	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 8.1-28.5°C	W.Y. Shiu, D. Mackay
Salinity: 30 g(2)/kg sln	W.I. Shild, D. Mackay
EXPERIMENTAL VALUES:	
Solubility of 1-ethylnaph	thalene in 0.5 mol(2)/L sln
<u>t/°C</u>	10 ⁵ mol(1)/L sln
8.1	3.65
11.1	3.87
17.4 20.3	4.23 4.45
23.3	4.45
25.0	4.67
26.2 28.5	4.53 4.82
AUXILIARY	' INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	······································
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea-	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade - Water: distilled over a KMnO ₄ -
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl-	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade - Water: distilled over a KMnO ₄ - NaOH solution and passed
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade - Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade - Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade - Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and they its fluorescent intensity was mea-	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and they its fluorescent intensity was mea- sured at 365 nm. The Spectrofluori-	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade - Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and thei its fluorescent intensity was mea- sured at 365 nm. The Spectrofluori- meter employed a ratio-photon count- ing mode where 1-ethylnaphthalene	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade n ESTIMATED ERROR: Solubility ± 2.0% (author)
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and thei its fluorescent intensity was mea- sured at 365 nm. The Spectrofluori- meter employed a ratio-photon count- ing mode where 1-ethylnaphthalene concentration was linearly related to the fluorescence signal. The UV	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and ther its fluorescent intensity was mea- sured at 365 nm. The Spectrofluori- meter employed a ratio-photon count- ing mode where 1-ethylnaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorp	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 365 nm. The Spectrofluori- meter employed a ratio-photon count- ing mode where 1-ethylnaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorp- tivity of 1-ethylnaphthalene in eth- anol solution therefore provide an absolute solubility scale for the	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 365 nm. The Spectrofluori- meter employed a ratio-photon count- ing mode where 1-ethylnaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorp- tivity of 1-ethylnaphthalene in eth- anol solution therefore provide an	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)
METHOD/APPARATUS/PROCEDURE: The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence meth- od, saturated solution was prepared by adding excess amount of 1-ethyl- naphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 365 nm. The Spectrofluori- meter employed a ratio-photon count- ing mode where 1-ethylnaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorp- tivity of 1-ethylnaphthalene in eth- anol solution therefore provide an absolute solubility scale for the	SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Ethylnaphthalene; C₁₂H₁₂; [939-27-5] (2) Water; H₂O; [7732-18-5]</pre>	Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	· ·
The solubility of 2-ethylnaphthalene reported to be 8.00 mg(l)/kg(2) and 5	$.1 \times 10^{-5} mol(1) dm^{-3}(2)$ .
The corresponding mass percent and mo by the compiler are 8.00 x $10^{-4}$ g(l)/	le fraction, $x_1$ , calculated 100 g sln and 9.22 x 10 ⁻⁷ .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<ol> <li>source not specified; analytical grade; used as received; no impurities by glc.</li> <li>doubly distilled; free of trace organics.</li> </ol>
	ESTIMATED ERROR:
	<pre>temp. ± 0.5°C soly. ± 0.1 mg(1)/kg(2) (from eight determinations)</pre>
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2-Allyl-1,3,5-trimethylbenzene; C ₁₂ H ₁₆ ; [4810-05-3]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-40°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	L
Solubility of Water in 2-A	llyl-1,3,5-trimethylbenzene
<u>t/°C</u> <u>g(2)/100 g s</u>	$\frac{10^3 x_2 \text{ (compiler)}}{10^3 x_2 \text{ (compiler)}}$
20 0.0246	1.15
30         0.0331           40         0.0438	1.54 2.04
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hr. with (2). Next, calcium	(2) Not specified.
hydride was added and the evolving hydrogen volume measured and hence	(2) Not specified.
the concentration of (2) in (1) was evaluated.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

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COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Propyl-1,3,5-trimethylbenzene; C₁₂H₁₈; [4810-04-2]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-40°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Water in 2-Pro	py1-1,3,5-trimethylbenzene
<u>t/°C</u> g(2)/100 g sln	$10^3 x_2$ (compiler)
20       0.0255         30       0.0343         40       0.0455	2.29 3.08 4.09
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	<ul><li>(1) Not specified.</li><li>(2) Not specified.</li></ul>
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) l-Phenylhexane; C ₁₂ H ₁₈ ; [1077-16-3]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.
(2) Water; H ₂ O; [7732-18-5]	Vodnye. Resursy. <u>1975</u> , 2, 170-3.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-phenylhexane in water at 25°C was reported to be 0.0021 mg(1) cm ⁻³ sln. The corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are 0.00021 g(1)/100 g sln and 2.4 x 10 ⁻⁷ . The assumption that 1.00 L sln = 1.00 kg sln was used in the calculation.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc.	(1) described in ref (1).
A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G column operated at 90-140°C.	(2) distilled.
	ESTIMATED ERROR:
	temp. ± l°C
	REFERENCES:
	1. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya 1973, 13, 885.

COMPONENTS :	EVALUATOR:
<pre>(1) Dodecane; C₁₂H₂₆; [112-40-3] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	April 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the system dodecane (1) - water (2) have been reported in the publications listed in Table 1.

TABLE 1: Qua			
the Dodeo	cane (1) -	Water (2)	System

Reference	T/K	Solubility	Method
Schatzberg (ref l)	298,313	(2) in (1)	Karl Fischer
Franks (ref 2)	298	(l) in (2)	GLC
Sutton and Calder (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

### 1. SOLUBILITY OF DODECANE (1) IN WATER (2)

The solubility of dodecane in water has been reported in only two publications, both at 298K (Table 1). The agreement between the two studies is very poor with Franks value (ref 2) considerably higher than that reported by Sutton and Calder (ref 3). Support for the lower value comes from extrapolation of the lower n-alkane solubilities. However, there is sufficient uncertainty in this extrapolation to preclude rejection of the higher value at this time. The available data are summarized in Table 2.

TABLE 2: Tentative Solubility Values of Dodecane (1) in Water (2)

T/K	Solubility	values	
	Reported values 10 ⁷ g(1)/100g sln	"Best" value ^a 10 ⁷ g(1)/100g sln	10 ¹⁰ <i>x</i> 1
298	8.42 (ref 2), 3.7 (ref 3)	3.7	3.9

a Datum from ref 3 preferred as Tentative value; see text.

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(continued next page)

COMPONENTS :	EVALUATOR:
<pre>(1) Dodecane; C₁₂H₂₆; [112-40-3] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. April 1986.

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN DODECANE (1)

As only the data of Schatzberg (ref 1) are available no Critical Evaluation is possible. However, it may be noted that the values of Schatzberg in well characterized systems are generally reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

REFERENCES

- 1. Schatzberg, P. J. Phys. Chem. <u>1963</u>, 67, 776-9.
- 2. Franks, F. Nature (London) <u>1966</u>, 210, 87-8.
- 3. Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u>, 8, 654-7.

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COMPONENTS:		ORIGINAL MEASUREMENTS:	
(l) Dodec	ane; C ₁₂ H ₂₆ ; [112-40-3]	Schatzberg, P.	
(2) Water	; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.	
VARIABLES:		PREPARED BY:	
Temperatu	re: 25-40°C	M.C. Haulait-Pirson	
EXPERIMENTAL	VALUES:	· · · · · · · · · · · · · · · · · · ·	
	Solubility of wate	er in dodecane	
	t/°C mg(2)/k	$\frac{g sln}{2}$	
	25 65	$6.1 \times 10^{-4}$	
	40 127		
	^a See "Estimated Error"		
		INFORMATION	
<pre>(1) was s layer of without a was seale pletely s for 7 day withdrawn phobized bilized K to a tite used to t in the pr "dead-sto</pre>	ATUS/PROCEDURE: aturated by storing over a (2) in a brown glass bottle ny agitation. The bottle d with serum cap and com- ubmerged in the water-bath s. A 20-mL sample was with a silicone-hydro- hypodermic syringe. Sta- arl Fischer reagent diluted r of 1.0-1.3 mg(2)/mL was titrate (2) in (1) directly esence of methanol to a p" end-point using a F3 automatic titrimeter.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co.; pure grade; 99+ mole %; passed repeatedly through a column of silica gel until no absorp- tion occurred in the 220 to 340 nm spectral range. (2) distilled and deionized. ESTIMATED ERROR: temp. ± 0.02°C soly. a) 0-6%; b) 0-2% (deviations from the mean) REFERENCES:</pre>	

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3]	Franks, F.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) <u>1966</u> , 210, 87-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of dodecane in water a in mole fraction $x_1 = 8.9 \times 10^{-10}$ . The corresponding mass percent calcul 8.42 $\times 10^{-7}$ g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator fitted to the chroma- tographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.	<ul> <li>(1) Fluka; purum grade; purity &gt; 97% (chromatographic analysis).</li> <li>(2) not specified.</li> </ul>
	ESTIMATED ERROR:
	soly. ± 12%
	REFERENCES :

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Dodecane; C₁₂H₂₆; [112-40-3] Sutton, C.; Calder, J.A. (2) Water; H₂O; [7732-18-5] Environ. Sci. Technol. 1974, 8, 654-7. VARIABLES: PREPARED BY: M.C. Haulait-Pirson One temperature: 25°C **EXPERIMENTAL VALUES:** The solubility of dodecane in water at 25°C was reported to be 3.7 x  $10^{-7}$  g(1)/100 g(2) corresponding to a mole fraction  $x_1$  of  $4 \times 10^{-10}$ . AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: (1) Analabs Inc., 99+%. 175 mg (1) were equilibrated with 700 mL (2) in closed flasks by sha-(2) doubly distilled. king on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane con-taining an internal standard. The concentration of (1) was determined by injection of the hexane extract ESTIMATED ERROR: into a dual column gas chromatograph equipped with flame ionization detemp. ± 0.1°C tectors. soly. ± 16% **REFERENCES:** 

COMPONENTS :	EVALUATOR:
<ul> <li>(1) Dodecane; C₁₂H₂₆; [112-40-3]</li> <li>(2) Seawater</li> </ul>	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

CRITICAL EVALUATION:

The solubility of dodecane (1) in seawater (2) at 298 K has been reported in three works:

Authors	Method	Salinity g salts/kg sln	10 ⁷ g(l)/100 g sln
Krasnoshchekova and Gubergrits (ref l)	GLC	6	5
Sutton and Calder (ref 2)	GLC	35	2.9
Button (ref 3)	isotopic	12	1.74

The reported data are all from different salinities which precludes direct comparison. Since the data are in only fair agreement with each other and with the reported values for the solubility of dodecane in pure water, all three values are adopted as tentative.

	SOLUBILITY OF	DODECANE (1) IN SEAWA	TER (2)
		TENTATIVE VALUE	
T/K		g salts/kg sln	g(l)/100 g sln
298		35	$2.9 \times 10^{-7}$

REFERENCES

- Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. Neftekhimiya, <u>1973</u>, 13, 885-8.
- 2. Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u>, 8, 654-7.
- 3. Button, D.K. Geochim. Cosmochim. Acta 1975, 40, 435-40.

382 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Dodecane; C₁₂H₂₆; [112-40-3] Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. (2) Seawater Neftekhimiya 1973, 13, 885-8. VARIABLES : PREPARED BY: One temperature: 25°C Salinity: 6 g/kg sln M. Kleinschmidt EXPERIMENTAL VALUES: The solubility of dodecane in seawater was reported to be  $5 \times 10^{-7}$  g(1)/100 g sln. and the corresponding mole fraction,  $x_1 = 5.0 \times 10^{-10}$ .

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: A saturated solution was prepared (1) "chemically pure" by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. (2) distilled water plus salt in a flask placed in a temperature controlled bath. A sample of solumixture. tion was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding ESTIMATED ERROR: solution concentration calculated. not specified. **REFERENCES**:

ORIGINAL MEASUREMENTS:
Sutton, C.; Calder, J.A.
Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
PREPARED BY:
P.A. Meyers and D. Shaw
er was reported to be .1 x 10 ⁻¹⁰ .
INFORMATION
SOURCE AND PURITY OF MATERIALS:
<pre>Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</pre> ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3]	Button, D. K.
(2) Salt mixture (ref 1)	Geochim. Cosmochim. Acta <u>1975</u> , 40, 435-40.
(3) Water; H ₂ O; [7732-18-5]	,
VARIABLES:	PREPARED BY:
One temperature: 25°C Constant salinity: 12 g(2)/kg sln Different periods of standing	P. Meyers and D. Shaw
EXPERIMENTAL VALUES:	·
gently stirring for 1	n in saline medium after week and then remaining the periods shown
<u>Time, Weeks</u>	Dodecane, $\mu g(1)/L(2)$
1 8 16	2.16 ± 0.03 1.80 ± 0.02 1.78 ± 0.02
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Dodecane solutions were prepared in a chemically defined solution resem- bling dilute seawater. In addition to the mineral salts and vitamins reported (ref 1), the solution con- tained 1 mg/L arginine and 10 g/L NaCl. After sterilization (121°C for 30 min), 0.8 µL of ¹⁴ C-dodecane was sprayed on to the medium surface to form a thin film. Gentle sub- surface agitation was induced by a 3 in magnet rotating at 60 rev/min	Amersham Searle Corp. (Arlington Heights, Ill.) supplied the [1- ¹⁴ C] dodecane, 27 µCi/µmol. It was ac- companied by a gas chromatogram of the preparation showing a single peak at the appropriate location.
against the inside carboy wall at midlevel. The subsurface dodecane concentration was determined from the radioactivity of samples col- lected from a port at the bottom	ESTIMATED ERROR: Experimental error is estimated at ± 1%.
of the carboy. The system was stirred for 1 week and then allowed to stand. Equilibrium appeared to have been achieved within 8 weeks.	REFERENCES: 1. Button, D. K. Limnol. Oceanogr. <u>1969</u> , 14, 95-100.

COMPONENTS:	EVALUATOR:
<pre>(1) Fluorene; C₁₃H₁₀; [86-73-7] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	April 1986.

CRITICAL EVALUATION:

Quantitative solubility data for fluorene (1) in water (2) have been reported in the publications listed in Table 1. No solubility data for water in fluorene have been reported.

TABLE 1:	Quantita	tive	Solubili	ty	Studies	of
	Fluorene	( <u>1)</u> i	In Water	(2)	_	

Reference	T/K	Method
Wauchope and Getzen (ref 1)	273-348	spectrophotometric
Mackay and Shiu (ref 2)	298	spectrofluorometric
May et al. (ref 3)	298	chromatographic

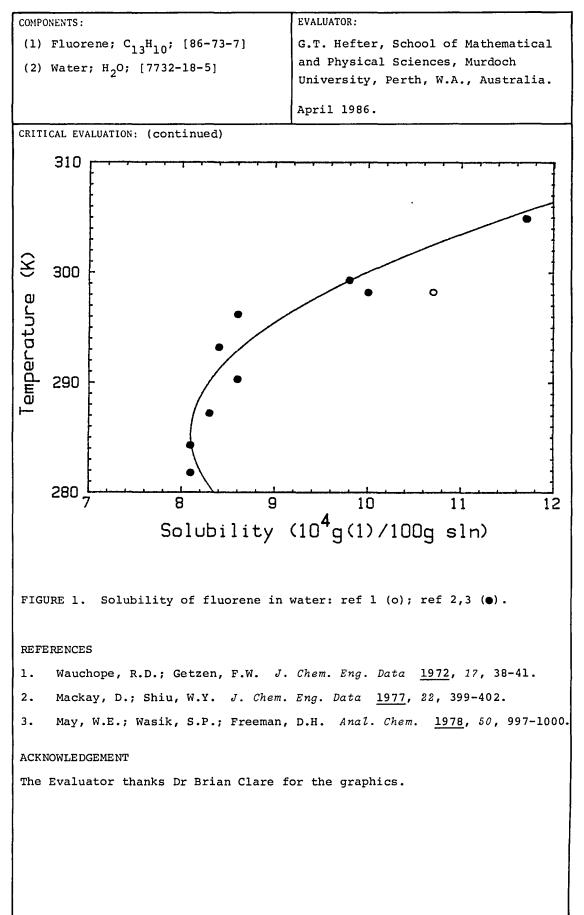
The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The solubility values are also summarized in Table 2 and plotted in Figure 1.

At 298K, the only temperature where comparison is possible, the available data (ref 1-3) are in good agreement and the average value can be Recommended. At other temperatures only the values of Wauchope and Getzen (ref 1) are available and are therefore regarded as tentative.

TABLE 2: Recommended (R) and Tentative Solubility Values ofFluorene (1) in Water (2)

T/K	Solubili	ty values	L
I	Reported values ^a	"Best" value	$es (t g_n)^p$
	10 ⁴ g(1)/100g sln	"Best" value 10 ⁴ g(l)/100g sln	10 ⁶ x1
273	0.66 (ref 1)	0.7	0.8
298	l.90 (ref 1), l.98 (ref 2), l.685 (ref 3)	$1.9 \pm 0.1 (R)$	2.1 (R)
303	2.4* (ref 1)	2.4	2.6
313	3.8* (ref 1)	3.8	4.1
323	6.29 (ref 1)	6.3	6.8
333	10.4* (ref 1)	10	11
343	18.5* (ref 1)	19	21
ł			

a Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the authors' original values.
 b Obtained by averaging where appropriate; σ_n has no statistical significance.
 (continued next page)



chope, R.D.; Getzen, F.W.
Chem. Eng. Data <u>1972</u> , 17, 8-41.
ARED BY: Maczynski
4

### EXPERIMENTAL VALUES:

## Solubility of fluorene in water

	mg(1)/kg(	2)	٨	7
t/°C		smoothed with	10 ⁴ g(1)/100 g sln	$10^{7}x_{1}$
	experiment	(std dev)	(compiler)	(compiler)
0.0		0.66(0.01)	0.66	7.2
24.6	1.93, 1.87, 1.88	1.86	1.86	20.2
25.0		1.90(0.03)	1.90	20.6
29.9	2.41, 2.33, 2.34	2.37	2.37	25.7
30.3	2.10, 2.25, 2.23	2.41	2.41	26.1
38.4	3.72, 3.73	3.53	3.53	38.2
40.1	3.88, 3.84, 3.85	3.84	3.84	41.6
47.5	5.59, 5.62, 5.68	5.54	5.54	60.0
50.0		6.29(0.05)	6.29	68.2
50.1	6.31, 6.42, 6.54	6.32	6.32	68.5
50.2	6.27	6.35	6.35	68.8
54.7	8.31, 8.41, 8.56	8.02	8.02	86.9
59.2	10.5, 10.5	10.2	10.2	110
60.5	10.7, 11.0, 11.6	10.9	10.9	118
65.1	14.2, 14.1, 14.2	14.1	14.1	153
70.7	18.5, 18.5, 18.9	19.3	19.3	209
71.9	18.8	20.6	20.6	223
73.4	21.5	22.5	22.5	244
75.0		24.7(0.4)	24.7	268

AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE: Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glass- ware.	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.</li> <li>(2) distilled and deionized.</li> </ul>
	<pre>temp. ± 0.5°C soly. see experimental values     above REFERENCES:</pre>

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ORIGINAL MEASUREMENTS:
COMPONENTS:
 (1) Fluorene; C<sub>13</sub>H<sub>10</sub>; [86-73-7]
 Mackay, D.; Shiu, W.Y.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
 J. Chem. Eng. Data <u>1977</u>, 22,
 399-402.
VARIABLES:
 PREPARED BY:
 One temperature: 25°C
 M.C. Haulait-Pirson
EXPERIMENTAL VALUES:
 The solubility of fluorene in water at 25°C was reported
 to be 1.98 mg(1) dm<sup>-3</sup> sln and x_1 = 2.14 \times 10^{-7}.
 The corresponding mass percent calculated by the compiler
 is 1.98 \times 10^{-4} g(1)/100 g sln.
 AUXILIARY INFORMATION
 SOURCE AND PURITY OF MATERIALS:
METHOD / APPARATUS / PROCEDURE :
 A saturated solution of (1) in (2)
 (1) Aldrich Chemicals, Eastman
 was vigorously stirred in a 250 mL
 Kodak, or K and K Laboratories,
 flask for 24 hrs. and subsequently
 commercial highest grade;
 settled at 25°C for at least 48 hrs.
 used as received.
 Then the saturated solution was
 decanted and filtered and 50-100 mL
 (2) doubly distilled.
 extracted with approximately 5 mL
 of cyclohexane in a separatory
funnel. After shaking for 2 hrs.
 the cyclohexane extract was removed
 for analysis.
 An Aminco-Browman
 spectrophotofluorometer (American
 Instruments Ltd.) was used for
 ESTIMATED ERROR:
 analysis. Many details are given
 soly. \pm 0.04 mg(l) dm<sup>-3</sup> sln
 in the paper.
 (maximum deviation from several
 determinations.)
 REFERENCES:
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1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]       May, W.E.; Wasik, S.P.; Freeman, D.         2) Water; H ₂ O; [7732-18-5]       Anal. Chem. <u>1978</u> , 50, 997-1000.         RTABLES:       PREPARED BY:         An action of the corresponding mass percent and mole fraction, x ₁ , values calculated y compiler are 1.685 x 10 ⁻⁴ g(1)/100 g sln and 1.826 x 10 ⁻⁷ .         XIXILIAN INFORMATION         ZHOD/APPARATUS/PROCEDURE:         he dynamic coupled column liquid hromatography (DCCLC) method was ased on generating saturated solumions by pumping water through a lolumn packed with the component is generator column). The conentration of (1) in the effluent f the generator column). The conentration of (1) in the effluent f the generator column as mearured by a modification of the oupled column liquic chromato-	COMPONENTS :	ORIGINAL MEASUREMENTS:
2) Water; H ₂ O; [7732-18-5]       Anal. Chem. <u>1978</u> , 50, 997-1000.         RTABLES:       PREPARED BY:         Anal. Chem. <u>1978</u> , 50, 997-1000.         RTABLES:       PREPARED BY:         A. Maczynski         FFEIMENTAL VALUES:         The solubility of fluorene in water at 25°C was reported to be        665 mg(1)/kg(2).         he corresponding mass percent and mole fraction, x ₁ , values calculated y compiler are 1.685 x 10 ⁻⁴ g(1)/100 g sln and 1.826 x 10 ⁻⁷ .         AUXILIARY INFORMATION         THOD/AFPARATUS/FROCEDURE:         he dynamic coupled column liquid hromatography (DCCLC) method was ased on generating saturated solumin packed with glass beads that we been coated with the component 1) (generator column). The conentration of (1) in the effluent f the generator column). The conentration of (1) in the effluent f the generator column liquid chromato-raphic process that has been         SUMMER SERVE         SUMER AND PURITY OF MATERIALS:         (2) distilled over KMNO, and NAOH and passed through a column packed with Apple process that has been		ORIGINAL MERSUREMIS:
INTABLES:       PREPARED BY:         A. Maczynski         PPERIMENTAL VALUES:         the solubility of fluorene in water at 25°C was reported to be         .685 mg(1)/kg(2).         the corresponding mass percent and mole fraction, x1, values calculated         by compiler are 1.685 x 10 ⁻⁴ g(1)/100 g sln and 1.826 x 10 ⁻⁷ .         AUXILIARY INFORMATION         THOD/AFPARATUS/FROCEDURE:         he dynamic coupled column liquid         hromatography (DCCLC) method was         ased on generating saturated solutions by pumping water through a         olumn packed with glass beads that         10 (generator column). The contentration of (1) in the effluent         f the generator column). The content the generator column liquid chromato-         f the generator column liquid chromato-         raphic process that has been         Structure tensore	(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]	May, W.E.; Wasik, S.P.; Freeman, D.H.
A. Maczynski         PERIMENTAL VALUES:         the solubility of fluorene in water at 25°C was reported to be         .685 mg(1)/kg(2).         the corresponding mass percent and mole fraction, x ₁ , values calculated or compiler are 1.685 x 10 ⁻⁴ g(1)/100 g sln and 1.826 x 10 ⁻⁷ .         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         the dynamic coupled column liquid hromatography (DCCLC) method was ased on generating saturated solutions by pumping water through a column packed with thas been that ave been coated with the component 1) (generator column). The con-entration of (1) in the effluent f the generator column was mea-ured by a modification of the goupled column liquid chromato-raphic process that has been	(2) Water; H ₂ O; [7732-18-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.
A. Maczynski         PERIMENTAL VALUES:         the solubility of fluorene in water at 25°C was reported to be         .685 mg(1)/kg(2).         the corresponding mass percent and mole fraction, x ₁ , values calculated or compiler are 1.685 x 10 ⁻⁴ g(1)/100 g sln and 1.826 x 10 ⁻⁷ .         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         the dynamic coupled column liquid hromatography (DCCLC) method was ased on generating saturated solutions by pumping water through a column packed with thas been that ave been coated with the component 1) (generator column). The con-entration of (1) in the effluent f the generator column was mea-ured by a modification of the goupled column liquid chromato-raphic process that has been	WADTABIES.	DEPARED DV.
PERIMENTAL VALUES:         The solubility of fluorene in water at 25°C was reported to be         .685 mg(1)/kg(2).         the corresponding mass percent and mole fraction, $x_1$ , values calculated y compiler are 1.685 x 10 ⁻⁴ g(1)/100 g sln and 1.826 x 10 ⁻⁷ .         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         the dynamic coupled column liquid hromatography (DCCLC) method was ased on generating saturated solutions by pumping water through a column packed with the component 1) (generator column). The conentration of (1) in the effluent f the generator column was mearmer been coated with the component f the generator column was mearmer been column liquid chromatography (DCCLC) method was mearmer been coated with the component f the generator column was mearmer been coated with the component f the generator column was mearmer been coated with the component f the generator column was mearmer been coated with the been coated with the been coated with the been coated with the component f the generator column was mearmer been coated with the component f the generator column was mearmer been coated with the been been coated with the been been been been been bead been bead		
AUXILIARY INFORMATION         AUXILIARY INFORMATION         AUXILIARY INFORMATION         Stress         THOD/APPARATUS/PROCEDURE:         he dynamic coupled column liquid hromatography (DCCLC) method was ased on generating saturated solu- ions by pumping water through a olumn packed with the component 1) (generator column). The con- entration of (1) in the effluent f the generator column was mea- ured by a modification of the oupled column liquid chromato- raphic process that has been	One temperature: 25°C	A. Maczynski
AUXILIARY INFORMATION         AUXILIARY INFORMATION         ETHOD/APFARATUS/PROCEDURE:         the dynamic coupled column liquid hromatography (DCCLC) method was ased on generating saturated solu- ions by pumping water through a olumn packed with glass beads that ave been coated with the component 1) (generator column) The con- entration of (1) in the effluent f the generator column was mea- ured by a modification of the oupled column liquid chromato- raphic process that has been       Source AND PURITY OF MATERIALS: (1) commercial product; less than 3% impurities. (2) distilled over KMnO4, and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).	EXPERIMENTAL VALUES:	
<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) commercial product; less than 3% impurities.</li> <li>(2) distilled over KMnO₄ and NaOH and passed through a column packed with glass beads that ave been coated with the component</li> <li>(1) commercial product; less than 3% impurities.</li> <li>(2) distilled over KMnO₄ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).</li> <li>Father of the oupled column liquid chromatorraphic process that has been</li> </ul>		
<ul> <li>the dynamic coupled column liquid hromatography (DCCLC) method was ased on generating saturated solutions by pumping water through a olumn packed with glass beads that ave been coated with the component 1) (generator column). The contentration of (1) in the effluent f the generator column was meatured by a modification of the oupled column liquid chromatorraphic process that has been</li> <li>(1) commercial product; less that 3% impurities.</li> <li>(2) distilled over KMnO₄ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).</li> </ul>	AUXILIARY	/ INFORMATION
<ul> <li>hromatography (DCCLC) method was ased on generating saturated solutions by pumping water through a olumn packed with glass beads that ave been coated with the component 1) (generator column). The conentration of (1) in the effluent f the generator column was meaured by a modification of the oupled column liquid chromatorraphic process that has been</li> <li>than 3% impurities.</li> <li>(2) distilled over KMnO₄ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).</li> </ul>	METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
orgribod in rof ]	The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the coupled column liquid chromato- graphic process that has been	<pre>than 3% impurities. (2) distilled over KMnO₄ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).</pre>
		ESTIMATED ERROR:

temp. ± 0.05°C
soly. ± 0.005 mg(1)/100 kg(2)
 (standard deviation)

**REFERENCES:** 

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci. <u>1975</u>, 13, 535.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]	May, W.E.; Wasik, S.P.; Freeman, D.H.	
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.	
(3) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
One temperature: 25°C		
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay	
EXPERIMENTAL VALUES:		
The solubility of fluorene in aqueou	ns sodium chloride is	
reported in terms of the Setschenow	equation:	
$\log(S_0/S) = K_s C_s$		
where;		
S is the solubility	of (1) in water (mg/L)	
	of (l) in saline solution (mg/L)	
K _s is the Setschenow		
5	on of sodium chloride (mol/L)	
evaluating the equation for S over t	the range of $C_{s}^{0-0.7 \text{ mol/L}}$ ,	
$K_{s} = 0.267$ with $S_{o} = 1.685$ .		
35 g(2)/kg sln calculated by the compilers are 1.20 x $10^{-4}$ g(1)/100 g sln and 1.30 x $10^{-7}$ .		
AUXILIARY	INFORMATION	
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
A saturated solution of (1) was	(1) greater than 97% pure.	
prepared by pumping salt water through a "generation column" which	(2) reagent grade.	
was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C ₁₈ stationary phase, then a water- acetonitrile solvent was passed through for extraction. The extract was introduced into a	(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.	
liquid chromatograph and the concen-		
tration of (1) was measured with a UV detector.	temp ± 0.05°C	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Diphenylmethane; C₁₃H₁₂; [101-81-5] (2) Water; H₂O; [7732-18-5]</pre>	Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
VARIABLES :	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of diphenylmethane in 1.41 x 10 ⁻⁴ g(1)/100 g sln. The corresponding mole fraction, $x_1$ , is 1.51 x 10 ⁻⁷ .	
· · · · · · · · · · · · · · · · · · ·	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a mea- sured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorb- ance of the hexane phase was mea- sured against a hexane blank on the	<ol> <li>Eastman Kodak Co., best grade; purified by fractional freezing; m.p. 25°C.</li> <li>not specified.</li> </ol>
Beckman spectrophotometer.	ESTIMATED ERROR:
	not specified.
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4,5-Trimethylnaphthalene;	Mackay, D.; Shiu, W.Y.
$C_{13}H_{14}; [213-41-1]$	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
	thalene in water at 25°C was reported
to be 2.1 mg(1) dm ⁻³ sln and $x_1 = 2.1$	$5 \times 10^{-7}$ .
The corresponding mass percent calcul	ated by the compiler
is $2.1 \times 10^{-4}$ g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;
A saturated solution of (1) in (2)	(1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently	Kodak, or K and K Laboratories, commercial highest grade;
settled at 25°C for at least 48 hrs. Then the saturated solution was	used as received.
decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. $\pm$ 0.1 mg(1) dm ⁻³ sln
In the paper.	(maximum deviation from several determinations).
	REFERENCES:
	1

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) (2-Ethylcyclopentyl) benzene; C ₁₃ H ₁₈ ; [4810-07-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Water in (2-	Ethylcyclopentyl) Benzene
<u>t/°C</u> <u>g(2)/100 g sl</u>	$10^3 x_2$ (compiler)
10         0.0103           20         0.0168           30         0.0273	1.00 1.62 2.64
METHOD /APPARATUS / PROCEDURE :	INFORMATION
	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	<ul><li>(1) Not specified.</li><li>(2) Not specified.</li></ul>
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Cyclopentyloctane; C ₁₃ H ₂₆ ; [4810-01-9]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES :	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of Water in	n 2-Cyclopentyloctane
<u>t/°C</u> <u>g(2)/100 g s</u>	$\frac{10^4 x_2 \text{ (compiler)}}{2}$
10 0.0048	4.86
20 0.0075 30 0.0122	7.59 12.34
	· · · · · · · · · · · · · · · · · · ·
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hours with (2). Next, calcium	(2) Not specified.
hydride was added and the evolving	
hydrogen volume measured and hence the concentration of (2) in (1) was	
evaluated.	
	ESTIMATED ERROR:
	LOTINALED ERROR:
	Not specified.
	REFERENCES :

	395
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Tridecane; C ₁₃ H ₂₈ ; [629-50-5]	Schatzberg, P.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.
2	
VARIABLES:	PREPARED BY:
Temperature: 25-40°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of wate	
t/°C mg(2)/	$\frac{kg sln}{2}$
25 60	
40 123	b $12.6 \times 10^{-4}$
a See "Estimated Error"	
See Estimated Ellor	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was saturated by storing over a	(1) Phillips Petroleum Co.; research grade; 99.73 mole %; passed
layer of (2) in a brown glass bottle without any agitation. The bottle	repeatedly through a column
was sealed with serum cap and com- pletely submerged in the water-bath	of silica gel until no absorp- tion occurred in the 220 to
for 7 days. A 20-mL sample was withdrawn with a silicone-hydro-	340 nm spectral range.
phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted	(2) distilled and deionized.
to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly	ESTIMATED ERROR:
in the presence of methanol to a	temp. $\pm 0.02$ °C
"dead-stop" end-point using a Beckman KF3 automatic titrimeter.	soly. a) 0-6%; b) 0-2% (deviations from the mean)
	REFERENCES :

COMPONENTS: (1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Water; H₂O; [7732-18-5] EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in anthracene.

# TABLE 1: Quantitative Solubility Studies of Anthracene (1) in Water (2)

Reference	T/K	Method
Davis et al. (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Wauchope and Getzen (ref 3)	273-348	spectrophotometric
Mackay and Shiu (ref 4)	298	spectrofluorometric
Schwarz (ref 5)	282-305	spectrophotometric
May et al. (ref 6)	278-302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

With the exception of the 300K datum of Davis *et al.* (ref 1) which is several orders of magnitude lower than all other values, all the available data on the solubility of anthracene in water are summarized in Table 2. Selected data are also plotted in Figure 1.

At 298K the data are clustered around two values (Table 2). A possible explanation for this (ref 6) is that most commercial preparations of anthracene contain about 2% phenanthrene. Although isomeric with anthracene, phenanthrene is about 20 times more soluble which could result in higher observed values for analytical methods such as spectrophotometry which do not distinguish between the two isomers. However, at the present time there are insufficient data to justify rejection of the higher values. Clearly, a careful reinvestigation of this system is justified.

At temperatures lower than 298K the data of Schwarz (ref 5) and May  $et \ al.$  (ref 6) are in good agreement. However, in view of the discrepancies at 298K these values are regarded only as Tentative.

At T > 298K only the data of Wauchope and Getzen (ref 3) are available and in view of the disagreement at 298K must also be regarded as very tentative.

(continued next page)

		T	
COMPONENTS	5:	EVALUATOR:	
(l) Antl	hracene: C ₁₄ H ₁₀ ; [120-12-7]	G.T. Hefter, School of Ma	athematical
(2) Wate	er; H ₂ O; [7732-18-5]	and Physical Sciences, Mu	
	2	University, Perth, W.A.,	Australia.
		February 1986.	
CRITICAL E	EVALUATION: (continued)		
		ues of the Solubility of ) in Water (2)	
<i>Т/</i> К		blubility values	
	Reported values ^a	"Best" valu	
	10 ⁶ g(1)/100g sln	10 ⁶ g(1)/100g sln	10 ⁸ x1
273	2.2 (ref 3)	2.2	0.22
283	2.38* (ref 5), 1.74* (ref	$2.1 \pm 0.3$	0.21
293	3.48* (ref 5), 3.23* (ref		0.34
298	7.5 (ref 2), 7.5 (ref 3) 7.3 (ref 4), 4.46* (ref 5 4.46 (ref 6)	$6.2 \pm 1.5^c$	0.62°
303	8.0* (ref 3)	8 ^{<i>c</i>}	8 ^{<i>c</i>}
313	16* (ref 3)	16 ^{<i>c</i>}	16 <i>°</i>
323	28.6 (ref 3)	29 <i>°</i>	29 <i>°</i>
333	51* (ref 3)	51 <i>°</i>	51 <i>°</i>
343	91 (ref 3)	91 [°]	91 [°]
graphi b Obtair cance.	s masked by an asterisk (*) h ical interpolation of the aut ned by averaging where approp ext however.	hors' original data.	
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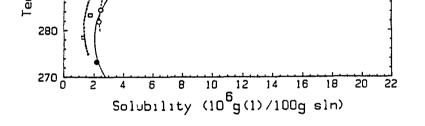


FIGURE 1. Solubility of anthracene in water, selected data: ref 3 ( $\bullet$ ), solid curve; ref 5 (o), broken curve; ref 6 ( $\Box$ ), broken curve.

COMPONENTS:	EVALUATOR:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	G.T. Hefter, School of Mathematical		
	and Physical Sciences, Murdoch		
(2) Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia.		
	February 1986.		
CRITICAL EVALUATION: (continued)			
REFERENCES			
<ol> <li>Davis, W.W.; Krahl, M.E.; Clove 108-10.</li> </ol>	es, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64,		
2. Klevens, H.B. J. Phys. Chem.	<u>1950</u> , <i>54</i> , 283-298.		
3. Wauchope, R.D.; Getzen, F.W. J	T. Chem. Eng. Data <u>1972</u> , 17, 38-41.		
4. Mackay, D.; Shiu, W.Y. J. Chem	n. Eng. Data <u>1977</u> , 22, 399-402.		
5. Schwarz, F.P. J. Chem. Eng. Da	nta <u>1977</u> , 22, 273-7.		
<ol> <li>May, W.E.; Wasik, S.P.; Freeman 1000.</li> </ol>	n, D.H. Anal. Chem. <u>1978</u> , 50, 997-		
ACKNOWLEDGEMENT			
The Evaluator thanks Dr Brian Clare	for the graphics.		
The Boardacor change br brian crare	ior the graphics.		

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Water; H₂0; [7732-18-5]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility	of	anthracene	in	water
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t/°C	$10^7 g(1) L^{-1} (2)$
27	7.5 ± 0.8
	7.2 ± 0.5
	7.5 ± 0.5

The best value recommended by the authors is 7.5 x  $10^{-7}$  g(1) L⁻¹ (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding values of mass percent and mole fraction,  $x_1$ , calculated by the compiler are 7.5 x  $10^{-8}$  g(1)/100 g sln and 7.6 x  $10^{-11}$ .

AUXILIARY INFORMATION			
ME THOD/APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	<ul> <li>(1) Eastman Kodak Company, 450x; m.p. range 215.6-216.5°C; used as received; (cf. ref 2).</li> <li>(2) dust-free.</li> </ul>		
	ESTIMATED ERROR:		
	temp. ± 3°C soly. see above.		
	<pre>REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V.     J. Am. Chem. Soc. 1942, 64,     101. 2. Davis, W.W.; Krahl, M.E.; Cloves,     G.H.A. J. Am. Chem. Soc.     1940, 62, 3086.</pre>		

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of anthracene in water	at 25°C was reported to be
$7.5 \times 10^{-5}$ g(1) dm ⁻³ sln and 4.47 x 1	$.0^{-7}$ mol(1) dm ⁻³ sln.
Assuming that 1.00 $dm^3$ sln = 1.00 $dm^3$	
and mole fraction, $x_1$ , calculated by	the compiler are 7.5 x $10^{-6}$ g(l)/
100 g sln and 8.07 $\times$ 10 ⁻⁹ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts	(1) not specified.
of (1) in 1 liter of (2) for as long	(2) not specified.
as three months. Aliquots were removed and concentrations deter-	
mined by spectra.	
	ESTIMATED ERROR:
	not specified
	not specified.
	REFERENCES :
1	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.
VARIABLES:	PREPARED BY:
Temperature: 0-75°C	A. Maczynski

EXPERIMENTAL VALUES:

## Solubility of anthracene in water

t/°C	mg(l)/kg(2)	moothed with	10 ⁵ g(1)/100 g sln	10 ⁸ x1
		(std dev)	(compiler)	(compiler)
0.0		0.022(0.001)	0.22	0.22
25.0		0.075(0.002)	0.75	0.76
35.4	0.125, 0.122, 0.119	0.123	1.23	1.24
39.3	0.152, 0.151, 0.148	0.159	1.59	1.61
44.7	0.208, 0.210, 0.206	0.214	2.14	2.16
47.5	0.279	0.249	2.49	2.52
50.0		0.286(0.003)	2.86	2.89
50.1	0.301, 0.297, 0.302	0.288	2.88	2.91
54.7	0.391, 0.389, 0.402	0.372	3.72	3.76
59.2	0.480, 0.488, 0.525	0.481	4.81	4.86
64.5	0.72, 0.62, 0.64	0.66	6.6	6.7
65.1	0.67, 0.64, 0.67	0.68	6.8	6.9
69.8	0.92	0.90	9.0	9.1
70.7	0.90, 0.97, 0.96	0.95	9.5	9.6
71.9	0.91	1.02	10.2	10.3
74.7	1.19, 1.13, 1.26	1.21	12.1	12.2
75.0	,,	1.23(0.02)	12.3	12.4
				<u> </u>

### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from One to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete	<ol> <li>Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.</li> <li>distilled and deionized.</li> </ol>
extraction.	ESTIMATED ERROR:
Standard solutions were prepared either by direct weighing using a	temp. ± 0.5°C
Cahn electrobalance, or by weighing	soly. see experimental values
0.1-0.2 g of samples followed by serial dilution in calibrated glass-	above
ware.	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	 
The solubility of anthracene in water	at 25°C was reported
to be 0.073 mg(1) dm ⁻³ sln and $x_1 = 7$	
<b>_</b>	1
The corresponding mass percent calcul is 7.3 x $10^{-6}$ g(1)/100 g sln.	ated by the compiler
15 7.3 X IU 9(I)/IUU 9 5IN.	
AUXILIARY INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed	(2) doubly distilled.
for analysis. An Aminco-Browman spectrophotofluorometer (American	
Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	<pre>soly. ± mg(1) dm⁻³ sln (maximum deviation from several determinations.)</pre>
	REFERENCES :

	403
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Schwarz, F.P.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data, 1977, 22, 273-7.
	· · · · · · · · · · · · · · · · · · ·
VARIABLES:	PREPARED BY:
Temperature: 8.6 - 31.3°C	A. Maczynski
EXPERIMENTAL VALUES:	
Solubility of Ant	
$t/^{\circ}C$ 10 ⁷ mol(1) L ⁻¹ 10 ⁶	$g(1)/100g sln = 10^9 x_1$
$\frac{t/^{\circ}C}{8.6} \qquad \frac{10' \text{ mol}(1) \text{ L}^{-1}}{1.31 \pm 0.04}$	<u>(compiler)</u> (compiler) 2.33 2.36
11.1 1.37 ± 0.03	2.44 2.47
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2.57 2.59 2.74 2.77
15.5 1.66 ± 0.03	2.96 3.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3.23 3.26 3.96 4.00
$23.0$ $2.34 \pm 0.03$	4.17 4.21
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccc} 4.10 & 4.14 \\ 4.10 & 4.14 \\ \end{array}$
26.2 2.67 ± 0.03	4.76 4.81
28.5         3.25         ±         0.06           31.3         3.90         ±         0.02	5.79 5.85 6.95 7.02
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Two methods were used. At 25°C the	(1) Source not specified; better
solubility of (1) in (2) was deter-	than 99 mole %, by glc, used
mined from UV absorption measurements and was used as a standard at other	as received.
temperatures. At other temperatures the spectrofluorimetry method was	(2) Distilled over KMnO ₄ and NaOH and passed through ⁴ a Sephadex
used. The sealed fluorescence cells	column.
contained 5 mL of the aqueous solu- tion and an excess of (1) were	
rotated at least 74 h in a water bath,	
then removed, quickly wiped dry and placed in the fluorimeter.	
	ESTIMATED ERROR:
	Temperature: ±0.1°C
	Solubility: See above.
	REFERENCES :
	L

-

COMPONENTS:

ORIGINAL MEASUREMENTS: (1) Anthracene; C₁₄H₁₀; [120-12-7] May, W.E.; Wasik, S.P.; Freeman, D.H. (2) Water; H₂O; [7732-18-5] Anal. Chem. 1978, 50, 175-9 and 997-1000. VARIABLES: PREPARED BY: Temperature: 5.2-29.0°C A. Maczynski EXPERIMENTAL VALUES: Solubility of anthracene in water 10⁹x1 10⁶ g(l)/100 g sln t/°C μg(1)/kg(2) (compiler) (compiler) 5.2  $12.7 \pm 0.4$ 1.27 1.28 10.0  $17.5 \pm 0.3$ 1.75 1.77 14.1 22.2 ± 0.1 2.22 2.24 18.3 29.1 ± 0.6 2.91 2.94 22.4 37.2 ± 1.1 3.72 3.76 24.6 43.4 ± 0.1 4.34 4.39 25.0 44.6 ± 0.2 4.46 4.51 28.7 55.7 ± 0.7 5.57 5.63 29.0 57.0 ± 3.0 5.7 5.76  $\mu g(1)/kg(2) = 8.21 + 0.8861 t + 0.0097 t^{2} + 0.0013 t^{3}$ AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The dynamic coupled column liquid (1) commercial product; less chromatography (DCCLC) method was based on generating saturated soluthan 3% impurities. (2) distilled over KMnO4 and NaOH tions by pumping water through a column packed with glass beads that and passed through a column have been coated with the component (1) (generator column). The conpacked with XAD-2 (Rohm and Hass, Philadelphia, Pa). centration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromato-ESTIMATED ERROR: graphic process that has been described in ref 1. temp. ± 0.05°C
soly. stand. dev. see above **REFERENCES**: 1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci. <u>1975, 13,</u> 535.

COMPONENTS:	EVALUATOR:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

CRITICAL EVALUATION:

The solubility of anthracene (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10 ⁶ g(1)/100 g sln
Schwarz (ref 1)	uv spectral	30	3.55
May et al. (ref 2)	HPLC	35.0	3.11

The reported data are from different salinities which precludes direct comparison. Since the data appear consistent with each other and with the tentative value for the solubility of anthracene in pure water, the data of Schwarz, and May *et al.* are adopted as tentative. Schwarz also reports data over the temperature range 281-303 K.

SOLUBILITY OF ANTHRACENE (1) IN SEAWATER (2) TENTATIVE VALUE

T/K	g salts/kg sln	10 ⁶ g(1)/100 g sln
298	35.0	3.11

### REFERENCES

- 1. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.
- May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

ORIGINAL MEASUREMENTS:	
Schwarz, F.P.	
J. Chem. Eng. Data <u>1977</u> , 22, 273-7.	
PREPARED BY:	
W.Y. Shiu, D. Mackay	
ne in 0.5 mol(2)/L	
$0^7 \text{ mol}(1)/\text{L sln}$	
0.93	
1.01 1.22	
1.47	
1.68 2.04	
1.92	
2.02 2.46	
AUXILIARY INFORMATION	
INFORMATION	
INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. ESTIMATED ERROR: Solubility ± 4.3 % (author) Temperature ± 0.1°C (author) REFERENCES:	

	407		
COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	May, W.E.; Wasik, S.P.; Freeman D.H.		
(2) Sodium Chloride; NaCl; [7647-14-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.		
(3) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
One temperature: 25°C			
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay		
EXPERIMENTAL VALUES:			
The solubility of anthracene in aqueous sodium chloride is			
reported in terms of the Setschenow	equation:		
$\log(S_{o}/S) = K_{s}C_{s}$			
where;			
S _o is the solubility	of (l) in water (mg/L)		
S is the solubility o	f (l) in saline solution (mg/L)		
K _s is the Setschenow	constant (L/mol)		
C _s in the concentration	on of sodium chloride (mol/L)		
evaluating the equation for S over t	he range of C $0-0.7$ (mol/L)		
$K_{\rm g} = 0.238$ with $S_{\rm o} = 0.0446$ .			
The corresponding mass percent and mole fraction $x_1$ , at salinity =			
$35 \text{ g}(2)/\text{kg}$ sin calculated by the compilers are $3.11 \times 10^{-6} \text{ g}(1)/\text{kg}$ sin			
and $3.22 \times 10^{-9}$ .			
AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
A saturated solution of (1) was	(1) greater than 97% pure.		
prepared by pumping salt water through a "generation column" which	(2) reagent grade.		
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium		
saturated solution was extracted with an "extractor column" packed	permanganate-sodium hydroxide and passed through an XAD-2		
with a superficially porous bonded	column.		
C ₁₈ stationary phase, then a water- acetonitrile solvent was passed			
through for extraction. The extract was introduced into a			
liquid chromatograph and the concen-	ESTIMATED ERROR:		
tration of (1) was measured with a UV detector.	temp ± 0.05°C K _s ± 0.004		
	s s ± 0.0002		
	REFERENCES:		

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COMPONENTS:

(1) Phenanthrene; C<sub>14</sub>H<sub>10</sub>; [85-01-8]

(2) Water; H<sub>2</sub>O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical

and Physical Sciences, Murdoch

University, Perth, W.A., Australia.

February 1986.
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CRITICAL EVALUATION:

Quantitative solubility data for phenanthrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported for the solubility of water in phenanthrene.

TABLE 1: Ouantitative Solubility Studies of

Phenanthr	cene (1) in Wate	<u>r (2)</u>
Reference	T/K	Method
Davis <i>et al</i> . (ref 1)	300	nephelometric
Andrews and Keefer (ref 2)	298	spectrophotometric
Klevens (ref 3)	298	spectrophotometric
Wauchope and Getzen (ref 4)	273-348	spectrophotometric
Eganhouse and Calder (ref 5)	298	GLC
Mackay and Shiu (ref 6)	298	spectrofluorometric
Schwarz (ref 7)	282-305	spectrofluorometric
May et al. (ref 8)	282-303	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The plethora of values reported (Table 1) at 298K for the solubility of phenanthrene (1) in water (2) enable a particularly critical assessment to be made. Thus the values of Davis *et al.* (ref 1) at 300K and of Klevens (ref 3) have been rejected as they are significantly higher than all other values. The remaining data at 298K are in good agreement enabling the average value to be Recommended.

At other temperatures where comparison is possible the data of May *et al.* (ref 8), Schwarz (ref 7) and Wauchope and Getzen (ref 4) are in excellent agreement enabling the average values to be Recommended over a reasonably wide range. At higher temperatures (> 303K) only the data of Wauchope and Getzen (ref 4) are available and must therefore be regarded as Tentative.

All the available data, except for the rejected values noted above (ref 1, 3), are summarized in Table 2 and plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) Phenanthrene; C₁₄H₁₀; [85-01-8] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

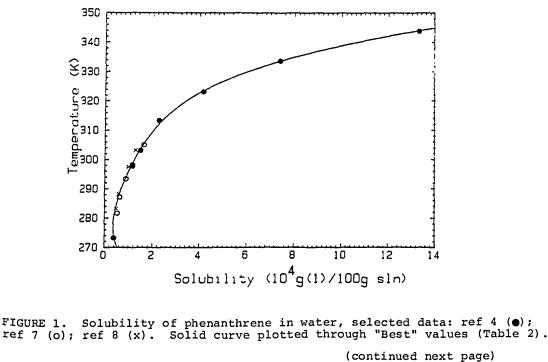
CRITICAL EVALUATION: (continued)

> Recommended (R) and Tentative Solubility Values of Phenanthrene (1) in Water (2) TABLE 2:

T/K	Solubility values				
	Reported values ^a	"Best	value:	s ( $\pm \sigma_n$ )	) ^b
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100	g sln	107	^x l
273	0.39 (ref 4)	0.4		0.4	
283	0.53* (ref 7), 0.46* (ref 8)	$0.50 \pm 0.0$	4 (R)	0.50	(R)
293	0.88* (ref 7), 0.78* (ref 8)	0.85 ± 0.0	5 (R)	0.86	(R)
298	0.994 (ref 2), 1.18 (ref 4), 1.07 (ref 5), 1.29 (ref 6), 1.151 (ref 7), 1.002 (ref 8)	1.1 ± 0.1	( <i>R</i> )	1.1	(R)
303	l.50* (ref 4), l.46* (ref 7), l.28* (ref 8)	1.4 ± 0.1	( <i>R</i> )	1.4	(R)
313	2.45* (ref 4)	2.5		2.5	
323	4.14 (ref 4)	4.1		4.1	
333	7.2* (ref 4)	7.2		7.2	
343	12.8* (ref 4)	13		13	
348	17 (ref 4)	17		17	

a Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the authors' original data.
b Obtained by averaging where appropriate; σ_n has no statistical signifi-

cance.



COMPO	DNENTS:	EVALUATOR:	
	Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.	
		February 1986.	
CRITI	CAL EVALUATION: (continued)		
REFE	ERENCES		
1.	<ol> <li>Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.</li> </ol>		
2.	Andrews, L.J.; Keefer, R.M. J.	Am. Chem. Soc. <u>1949</u> , 71, 3644-77.	
3.	Klevens, H.B. J. Phys. Chem. 1	950, 54, 283-298.	
4.	Wauchope, R.D.; Getzen, F.W. J.	Chem. Eng. Data <u>1972</u> , 17, 38-41.	
5.	Eganhouse, R.P.; Calder, J.A. G. 555-61.	eochim. Cosmochim. Acta <u>1976</u> , 40,	
6.	Mackay, D.; Shiu, W.Y. J. Chem.	Eng. Data <u>1977</u> , 22, 399-402.	
7.	. Schwarz, F.P. J. Chem. Eng. Data <u>1977</u> , 22, 273-7.		
8.	May, W.E.; Wasik, S.P.; Freeman, 1000.	D.H. Anal. Chem. <u>1978</u> , 50, 997-	
ACKN	NOWLEDGEMENT		
The	Evaluator thanks Dr Brian Clare for	or the graphics.	
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{			

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Phenanthrene; C₁₄H₁₀; [85-01-8] (2) Water; H₂0; [7732-18-5]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES: One temperature: 27°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of phe	nanthrene in water
t/°C	$10^3$ g(1) L ⁻¹ (2)
27	1.55
	1.62
	1.65

The best value recommended by the authors is  $1.60 \times 10^{-3}$  g(1) L⁻¹ (2). Assuming that 1.00 L sln = kg sln the corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 1.60 x  $10^{-4}$  g(1)/100 g sln and 1.62 x  $10^{-7}$ .

METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1. ESTIMATED ERROR: temp. ± 3°C
<pre>serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1. ESTIMATED ERROR: temp. + 3°C</pre>
temp. t 3°C
temp. ± 3°C
soly. $\pm 0.05 \times 10^{-3} g(1) dm^{-3}(2)$
REFERENCES:
1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc, <u>1942</u> , 64, 101.
2. Davis, W.W.; Krahl, M.E.; Clov
G.H.A. J. Am, Chem, Soc.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Water; H ₂ O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES: The solubility of phenanthrene in wat 9.94 x $10^{-5}$ g(1)/100 g sln. The corresponding mole fraction, $x_1$ , is 1.004 x $10^{-7}$ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a mea- sured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorb- ance of the hexane phase was mea- sured against a hexane blank on the Beckman spectrophotometer.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Eastman Kodak Co., best grade; recrystallized twice from ethanol; m.p. 101.0°C. (2) not specified.  ESTIMATED ERROR: not specified. REFERENCES:</pre>

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	L
The solubility of phenanthrene in wat 0.0016 x $10^{-5}$ g(1)/L sln and 9.0 x 10 Assuming that 1.00 dm ³ sln = 1.00 kg and mole fraction, $x_1$ , calculated by 100 g sln and 1.62 x $10^{-7}$ .	<pre>-6 mole (1)/L sln. sln the corresponding mass percent</pre>
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts	<ol> <li>not specified.</li> <li>act specified</li> </ol>
of (1) in 1 liter of (2) for as long as three months. Aliquots were	(2) not specified.
removed and concentrations deter- mined by spectra.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES :
L	L

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.
VARIABLES:	PREPARED BY:
Temperature: 0-75°C	A. Maczynski

#### EXPERIMENTAL VALUES:

ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete

Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by

serial dilution in calibrated glass-

extraction.

ware.

Solubility of phenanthrene in water								
t/°C	mg(l)/kg(	2) smoothed wit (std dev)	h 10 ⁴ g(l)/100 g sln (compiler)	$10^{7}x_{1}$ (compiler)				
0.0		0.39(0.01)	0.39	0.39				
24.6	1.12, 1.11	1.16 1.18(0.02)	1.16 1.18	1.17 1.19				
29.9	1.49, 1.49	1.49	1.49 1.52	1.51 1.54				
30.3 38.4	1.47, 1.48 2.44, 2.45	1.52 2.27	2.27	2.29				
40.1 47.5	2.27, 2.28, 2.25 3.81, 3.88, 3.87	2.47 3.63	2.47 3.63	2.50 3.67				
50.0	<b>·</b> • -	4.14(0.04)	4.14	4.18				
50.1 50.2	4.30, 4.38, 4.32 4.08, 4.04, 4.11	4.16	4.16 4.19	4.20 4.23				
54.7	5.66, 5.64, 5.63	5.34	5.34	5.40				
59.2 60.5			6.85 7.4	6.92 7.5				
65.1 70.7	9.8, 9.7, 9.8 12.4, 12.6, 12.4	9.6 13.3	9.6 13.3	9.7 13.4				
71.9	1.9 12.9 14.2		14.2	14.4				
73.4     18.2     15.6       75.0     17.2(0.3)			15.615.817.217.4					
AUXILIARY INFORMATION								
METHOD /	METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:							
Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from		lass- • The an open	(1) Baker reagent; recryst three times from ethe vacuum-sublimed twice purity not specified	er; e;				
one to three weeks between measure-			(2) distilled and deioni:	zed.				

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## ESTIMATED ERROR:

temp.	± 0.	.5°C	
soly.	see	experimental	values
	aboy	/e	

**REFERENCES:** 

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	415
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Phenanthrene; C₁₄H₁₀; [85-01-8] (2) Water; H₂0; [7732-18-5]</pre>	Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of phenanthrene in wat reported to be 1.07 mg(1)/kg(2) and 6 The corresponding mass percent and mo by the compiler are 1.07 x 10 ⁻⁴ g(1)/	$5 \times 10^{-6} \text{ mol(l) } \text{dm}^{-3}(2).$
METHOD /APPARATUS / PROCEDURE :	INFORMATION SOURCE AND PURITY OF MATERIALS:
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<pre>(1) source not specified; analytical grade; used as</pre>
	ESTIMATED ERROR:
	<pre>temp. ± 0.5°C soly. ± 0.01 mg(1)/kg(2) (from eight determinations)</pre>
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	· ·
The solubility of phenanthrene in wat to be 1.29 mg(1) dm ⁻³ sln and $x_1 = 1$ . The corresponding mass percent calcul is 1.29 x 10 ⁻⁴ g(1)/100 g sln.	$3 \times 10^{-7}$ .
15 1.29 x 10 g(1)/100 g sin.	
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American	<ul> <li>(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.</li> <li>(2) doubly distilled.</li> </ul>
Instruments Ltd.) was used for analysis. Many details are given	ESTIMATED ERROR: soly. $\pm$ 0.07 mg(1) dm ⁻³ sln
in the paper.	(maximum deviation from several determinations).
	REFERENCES :

(1) Phenanthrene: $C_{14}H_{10}$ ; $[85-01-8]$ Schwarz, F.P.(2) Water; $H_20$ ; $[7732-18-5]$ J. Chem. Eng. Data <u>1977</u> , 22,ARIABLES:PREPARED BY:Temperature: 8.4-31.8°CA. MaczynskiXPERIMENTAL VALUES:Solubility of phenanthrene in water $t'^{\circ}C$ $10^6 mol(1) L^{-1}$ $10^5 g(1)/100 g sln 10^8 (compiler)$ $8.4$ $2.81 \pm 0.07$ $5.01$ $8.4$ $2.81 \pm 0.07$ $5.01$ $11.1$ $3.09 \pm 0.07$ $5.51$ $14.0$ $3.59 \pm 0.06$ $6.40$ $17.5$ $4.40 \pm 0.04$ $7.84$ $22.2$ $4.94 \pm 0.09$ $8.80$ $23.3$ $6.09 \pm 0.07$ $10.85$ $25.0$ $6.46 \pm 0.02$ $11.51$ $25.0$ $6.46 \pm 0.02$ $11.51$ $21.3$ $7.7 \pm 0.2$ $13.72$ $31.8$ $9.13 \pm 0.08$ $16.27$ IGENTINGENTIONETHOD/APPARATUS/PROCEDURE:NOW methods were used.At 25°C the solubility of (1) in (2)was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.The sealed fluorescence cells colution and an excess of (1) were rotated at least 72 h in a water bath, then removed, guickly wipedESTIMATED ERKOR:	ONENTS .		ORIGINAL MEASUREMENTS:	·····	
(2) Water; H ₂ O; [7732-18-5]       J. Chem. Eng. Data <u>1977</u> , 22,         ARIABLES:       PREPARED BY:         Temperature: 8.4-31.8°C       A. Maczynski         XPERIMENTAL VALUES:       Solubility of phenanthrene in water         t/°C       10 ⁶ mol(1) L ⁻¹ 10 ⁵ g(1)/100 g sln <u>10⁸</u> (compiler)         8.4       2.81 ± 0.07       5.01       5.         11.1       3.09 ± 0.07       5.51       5.         14.0       3.59 ± 0.06       6.40       6.         7.5       4.40 ± 0.04       7.84       7.         20.2       4.94 ± 0.09       8.80       8.         23.3       6.09 ± 0.07       10.85       10.         25.0       6.46 ± 0.02       11.51       11.         29.3       7.7 ± 0.2       13.72       13.         31.8       9.13 ± 0.08       16.27       16.         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         Two methods were used.       Source AND PURITY OF MATERIALS:       (1) source not specified; bet than 9 molek, by glc?; used as received.         was determined from UV absorption measurements and was used.       Source AND PURITY OF MATERIALS:       (2) distilled over KMnOn, and 1 and passed through a Seph column.         Standard at oher tem	ONENTS:		URIGINAL MEASUREMENTS:		
ARIABLES: Temperature: $8.4-31.8^{\circ}$ C Solubility of phenanthrene in water $t/^{\circ}$ C $10^{6}$ mol(1) L ⁻¹ $10^{5}$ g(1)/100 g sln 10 ⁸ (compiler) (compiler) (compiler) (compiler) (c	Phenanthrene;	C ₁₄ H ₁₀ ; [85-01-8]	Schwarz, F.P.		
A. MaczynskiA. MaczynskiXPERIMENTAL VALUES:Solubility of phenanthrene in water $t/^{\circ}C$ $10^{6} mol(1) L^{-1}$ $10^{5} g(1)/100 g sln (compiler)$ $8.4$ $2.61 \pm 0.07$ $5.01$ $5.$ $11.1$ $3.09 \pm 0.07$ $5.51$ $5.$ $14.0$ $3.59 \pm 0.06$ $6.40$ $6.$ $17.5$ $4.40 \pm 0.09$ $8.80$ $8.$ $20.2$ $4.94 \pm 0.09$ $8.80$ $8.$ $23.3$ $6.09 \pm 0.07$ $10.85$ $10.$ $25.0$ $6.46 \pm 0.02$ $11.51$ $11.$ $29.3$ $7.7 \pm 0.2$ $13.72$ $13.$ $31.8$ $9.13 \pm 0.08$ $16.27$ $16.$ AUXILIARY INFORMATIONETHOD/APPARATUS/PROCEDURE:Two methods were used. $16.27$ $16.$ At 25°C the solubility of (1) in (2)was determined from UV absorption as used as standard at other temperatures. At other temperatures the spectrofluorimetry method was used. $(2)$ distilled over KMNO, and 1 and passed through a Seph column.The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were totated at least 72 h in a water totated at placed in the fluorimeter.ESTIMATED EROR: temp. $t 0.1^{\circ}C$ soly. see above	Water; H ₂ O; [	732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 273-7		
A. MaczynskiA. MaczynskiXPERIMENTAL VALUES:Solubility of phenanthrene in water $t/^{\circ}C$ $10^{6} mol(1) L^{-1}$ $10^{5} g(1)/100 g sln (compiler)$ $8.4$ $2.61 \pm 0.07$ $5.01$ $5.$ $11.1$ $3.09 \pm 0.07$ $5.51$ $5.$ $14.0$ $3.59 \pm 0.06$ $6.40$ $6.$ $17.5$ $4.40 \pm 0.09$ $8.80$ $8.$ $20.2$ $4.94 \pm 0.09$ $8.80$ $8.$ $23.3$ $6.09 \pm 0.07$ $10.85$ $10.$ $25.0$ $6.46 \pm 0.02$ $11.51$ $11.$ $29.3$ $7.7 \pm 0.2$ $13.72$ $13.$ $31.8$ $9.13 \pm 0.08$ $16.27$ $16.$ AUXILIARY INFORMATIONETHOD/APPARATUS/PROCEDURE:Two methods were used. $16.27$ $16.$ At 25°C the solubility of (1) in (2)was determined from UV absorption as used as standard at other temperatures. At other temperatures the spectrofluorimetry method was used. $(2)$ distilled over KMNO, and 1 and passed through a Seph column.The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were totated at least 72 h in a water totated at placed in the fluorimeter.ESTIMATED EROR: temp. $t 0.1^{\circ}C$ soly. see above		·····			
XPERIMENTAL VALUES:Solubility of phenanthrene in water $t/^{\circ}C$ $10^{6} mol(1) L^{-1}$ $10^{5} g(1)/100 g sln (compiler)$ $8.4$ $2.81 \pm 0.07$ $5.01$ $5.$ $11.1$ $3.09 \pm 0.07$ $5.51$ $5.$ $14.0$ $3.59 \pm 0.06$ $6.40$ $6.$ $20.2$ $4.94 \pm 0.09$ $8.80$ $8.$ $23.3$ $6.09 \pm 0.07$ $10.85$ $10.$ $25.0$ $6.46 \pm 0.02$ $11.51$ $11.$ $29.3$ $7.7 \pm 0.2$ $13.72$ $13.$ $31.8$ $9.13 \pm 0.08$ $16.27$ $16.$ Colspan="2">SOURCE AND FURITY OF MATERIALS:Two methods were used.AUXILIARY INFORMATIONETHOD/APPARATUS/PROCEDURE:Two methods were used.AUXILIARY INFORMATIONETHOD/APPARATUS/PROCEDURE:Colspan="2">SOURCE AND PURITY OF MATERIALS:Thom methods were used.AUXILIARY INFORMATIONETHOD/APPARATUS/PROCEDURE:Colspan="2">SOURCE AND PURITY OF MATERIALS:Thom methods were used.AUXILIARY INFORMATIONETHOD/APPARATUS/PROCEDURE:Thom methods were used.AL other temperatures.At other temperatures the spectrofluorimetry method was used.The sealed fluorescence cells colution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped 	ABLES:		PREPARED BY:		
Solubility of phenanthrene in water $\frac{t/^{\circ}C}{8.4} = \frac{10^{6} mol(1) t^{-1}}{2.81 \pm 0.07} = \frac{10^{5} g(1)/100 g sln}{(compiler)} = \frac{10^{8} (compiler)}{(compiler)} = \frac{(compiler)}{(compiler)} = $	nperature: 8.4-	1.8°C	A. Maczynski		
$t/^{\circ}C$ $10^{6} mol(1) L^{-1}$ $10^{5} g(1)/100 g sln (compiler)(compiler)8.42.81 ± 0.075.015.11.13.09 ± 0.075.515.14.03.59 ± 0.066.406.17.54.40 ± 0.047.847.20.24.94 ± 0.098.808.23.36.09 ± 0.0710.8510.25.06.46 ± 0.0211.5111.29.37.7 ± 0.213.7213.31.89.13 ± 0.0816.2716.VINITARY INFORMATIONAUXILIARY INFORMATIONAUXILIARY INFORMATIONAUXILIARY INFORMATIONAUXILIARY INFORMATIONAUXILIARY INFORMATIONContained 5 mL other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiged dry and placed in the fluorimeter.Source and pase during a Septice colspan="2">Solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiged dry and placed in the fluorimeter.ESTIMATED ERROR:temp. ± 0.1°C soly. see above$	RIMENTAL VALUES:			<u></u>	
(compiler)(compi8.42.81 ± 0.075.015.11.13.09 ± 0.075.515.14.03.59 ± 0.066.406.17.54.40 ± 0.047.847.20.24.94 ± 0.098.808.23.36.09 ± 0.0710.8510.25.06.46 ± 0.0211.5111.29.37.7 ± 0.213.7213.31.89.13 ± 0.0816.2716.Source and specified; betthan 99 molek, by glc;used as received.Xas determined from UV absorption(2) distilled over KMnO, and 1measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.(2) distilled over KMnO, and 1The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.ESTIMATED ERROR: temp. ± 0.1°C soly. see above		Solubility of ph	enanthrene in water		
AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         Two methods were used.         At 25°C the solubility of (1) in (2)         was determined from UV absorption         measurements and was used as a         standard at other temperatures.         At other temperatures the spectrofluorimetry method was used.         The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were totated at least 72 h in a water         bath, then removed, quickly wiped dry and placed in the fluorimeter.	°c —	10 ⁶ mol(1) L ⁻¹	10 ⁵ g(1)/100 g sln (compiler)	10 ⁸ x1 (compiler)	
A. 0 $3.59 \pm 0.06$ $6.40$ $6.$ $14.0$ $3.59 \pm 0.06$ $6.40$ $6.$ $17.5$ $4.40 \pm 0.04$ $7.84$ $7.$ $20.2$ $4.94 \pm 0.09$ $8.80$ $8.$ $23.3$ $6.09 \pm 0.07$ $10.85$ $10.$ $25.0$ $6.46 \pm 0.02$ $11.51$ $11.$ $29.3$ $7.7 \pm 0.2$ $13.72$ $13.$ $31.8$ $9.13 \pm 0.08$ $16.27$ $16.$ <b>AUXILIARY INFORMATIONETHOD/APPARATUS/PROCEDURE:</b> Two methods were used. $16.27$ At 25°C the solubility of (1) in (2)was determined from UV absorptionweasurements and was used as a standard at other temperatures.SOURCE AND PURITY OF MATERIALS: (1) source not specified; bet than 99 mole%, by glc; used as received.At other temperatures the spectrofluorimetry method was used.(2) distilled over KMnOu and 1 and passed through a Sephi column.The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were totated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.The sealed in the fluorimeter.ESTIMATED ERROR: temp. $\pm 0.1^{\circ}C$ soly. see above	. 4	2.81 ± 0.07	5.01	5.06	
AUXILIARY INFORMATION         AUXILIARY INFORMATION <td< td=""><td>.1</td><td>3.09 ± 0.07</td><td>5.51</td><td>5.57</td></td<>	.1	3.09 ± 0.07	5.51	5.57	
AUXILIARY INFORMATION         AUXILIARY INFORMATION <td< td=""><td>. 0</td><td>3.59 ± 0.06</td><td>6.40</td><td>6.47</td></td<>	. 0	3.59 ± 0.06	6.40	6.47	
23.3       6.09 ± 0.07       10.85       10.         25.0       6.46 ± 0.02       11.51       11.         29.3       7.7 ± 0.2       13.72       13.         31.8       9.13 ± 0.08       16.27       16.         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         EWo methods were used.       SOURCE AND PURITY OF MATERIALS:         At 25°C the solubility of (1) in (2)       vas determined from UV absorption         measurements and was used as a standard at other temperatures.       10 source not specified; bet than 99 mole%, by glc; used as received.         Standard at other temperatures.       (2) distilled over KMnO4, and 1 and passed through a Sepherofluorimetry method was used.         Che sealed fluorescence cells solution and an excess of (1) were rotated at least 72 h in a water path, then removed, quickly wiped try and placed in the fluorimeter.         ESTIMATED ERROR:         temp. ± 0.1°C soly. see above	. 5	$4.40 \pm 0.04$	7.84	7.92	
25.0       6.46 ± 0.02       11.51       11.         29.3       7.7 ± 0.2       13.72       13.         31.8       9.13 ± 0.08       16.27       16.         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         RWo methods were used.         At 25°C the solubility of (1) in (2)         Source and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.         ETHOD /APPARATUS/PROCEDURE:         Source and passed through a Sephator of the aqueous solution and an excess of (1) were cotated at least 72 h in a water path, then removed, quickly wiped try and placed in the fluorimeter.	. 2	4.94 ± 0.09	8.80	8.90	
29.3       7.7 ± 0.2       13.72       13.         31.8       9.13 ± 0.08       16.27       16.         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         SOURCE AND FURITY OF MATERIALS:         Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2"         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         Colspan="2">Colspan="2">Colspan="2">Colspan="2"         Colspan="2"	. 3	6.09 ± 0.07	10.85	10.97	
AUXILIARY INFORMATION AUXILIARY INFORMATION ETHOD/APPARATUS/PROCEDURE: EWO methods were used. At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. Che sealed fluorescence cells sontained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped kry and placed in the fluorimeter. AUXILIARY INFORMATION AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: (1) source not specified; bet than 99 mole%, by glc; used as received. (2) distilled over KMnOu, and 1 and passed through a Seph column. ESTIMATED ERROR: temp. ± 0.1°C soly. see above	. 0	6.46 ± 0.02	11.51	11.63	
AUXILIARY INFORMATION ETHOD/APPARATUS/PROCEDURE: EWo methods were used. At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells solution and an excess of (1) were cotated at least 72 h in a water bath, then removed, quickly wiped try and placed in the fluorimeter. AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: (1) source not specified; bet than 99 mole%, by glc; used as received. (2) distilled over KMnOu, and 1 and passed through a Seph column. ESTIMATED ERROR: temp. ± 0.1°C soly. see above	. 3	7.7 ± 0.2	13.72	13.87	
<ul> <li>ETHOD/APPARATUS/PROCEDURE:</li> <li>EWO methods were used.</li> <li>At 25°C the solubility of (1) in (2)</li> <li>Was determined from UV absorption</li> <li>measurements and was used as a</li> <li>standard at other temperatures.</li> <li>At other temperatures the</li> <li>Spectrofluorimetry method was used.</li> <li>Che sealed fluorescence cells</li> <li>contained 5 mL of the aqueous</li> <li>solution and an excess of (1) were</li> <li>cotated at least 72 h in a water</li> <li>bath, then removed, quickly wiped</li> <li>dry and placed in the fluorimeter.</li> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) source not specified; bet than 99 mole%, by glc;</li> <li>used as received.</li> <li>(2) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(2) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(2) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(3) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(4) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(5) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(6) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(7) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(8) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(9) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(1) source not specified; bet than 99 mole%, by glc;</li> <li>(2) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(1) source not specified; bet than 99 mole%, by glc;</li> <li>(2) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(2) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> <li>(3) distilled over KMnO4 and 1 and passed through a Sephacolum.</li> </ul>	. 8	9.13 ± 0.08	16.27	16.44	
<ul> <li>ETHOD/APPARATUS/PROCEDURE:</li> <li>Two methods were used.</li> <li>At 25°C the solubility of (1) in (2)</li> <li>was determined from UV absorption</li> <li>measurements and was used as a</li> <li>standard at other temperatures.</li> <li>At other temperatures the</li> <li>spectrofluorimetry method was used.</li> <li>The sealed fluorescence cells</li> <li>contained 5 mL of the aqueous</li> <li>solution and an excess of (1) were</li> <li>rotated at least 72 h in a water</li> <li>bath, then removed, quickly wiped</li> <li>dry and placed in the fluorimeter.</li> </ul>					
<ul> <li>Two methods were used.</li> <li>At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.</li> <li>(1) source not specified; bet than 99 mole%, by glc; used as received.</li> <li>(2) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(2) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(3) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(4) source not specified; bet than 99 mole%, by glc; used as received.</li> <li>(2) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(2) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(3) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(4) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(5) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(6) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(7) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(8) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(9) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> <li>(1) distilled over KMnO₄ and 1 and passed through a Sepher column.</li> </ul>		AUXILIARY	INFORMATION		
<ul> <li>At 25°C the solubility of (1) in (2)</li> <li>was determined from UV absorption</li> <li>measurements and was used as a</li> <li>standard at other temperatures.</li> <li>At other temperatures the</li> <li>spectrofluorimetry method was used.</li> <li>The sealed fluorescence cells</li> <li>contained 5 mL of the aqueous</li> <li>solution and an excess of (1) were</li> <li>rotated at least 72 h in a water</li> <li>bath, then removed, quickly wiped</li> <li>dry and placed in the fluorimeter.</li> </ul>	IOD/APPARATUS/PROCE	DURE :			
<pre>standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.</pre> and passed through a Seph column. ESTIMATED ERROR: temp. ± 0.1°C soly. see above	25°C the solub: determined from	lity of (1) in (2) om UV absorption	than 99 moles, by used as received.	glc;	
contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter. ESTIMATED ERROR: temp. ± 0.1°C soly. see above	measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.		and passed through a Sephadex		
rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter. ESTIMATED ERROR: temp. ± 0.1°C soly. see above	tained 5 mL of	the aqueous			
dry and placed in the fluorimeter. temp. ± 0.1°C soly. see above	solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.		ESTIMATED ERROR:		
REFERENCES :					
1			REFERENCES :	<u> </u>	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	May, W.E.; Wasik, S.P.; Freeman, D.H.
(2) Water; H ₂ O; [7732-18-5]	Anal. Chem. 1978, 50, 175-9 and
2	997-1000.
VARIABLES:	PREPARED BY:
Temperature: 8.5-29.9°C	A. Maczynski
EXPERIMENTAL VALUES:	
Colubility of p	econtbrono in victor
	henanthrene in water
t/°C μg(1)/kg(2)	$\frac{10^4 \text{ g(l)/100 g sln} \qquad 10^8 x_1}{(\text{compiler})}$
8.5 423 ± 4	0.423 0.427
10.0 468 ± 2	0.468 0.473
12.5 512 ± 1	0.512 0.517
15.0 601 ± 7	0.601 0.607
21.0 816 ± 8	0.816 0.825
24.3 995 ± 1	0.995 1.006
25.0 1002 ± 11	1.002 1.013
29.0 1220 ± 13	1.220 1.233
29.9 1277 ± 11	1.277 1.291
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the coupled column liquid chromato- graphic process that has been described in ref 1.	<ul> <li>(1) commercial product; less than 3% impurities.</li> <li>(2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).</li> <li>ESTIMATED ERROR: temp. ± 0.05°C soly. stand. dev. see above</li> <li>REFERENCES:</li> <li>1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci. 1975, 13, 535.</li> </ul>

COMPONENTS:	EVALUATOR:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

The solubility of phenanthrene (1) in seawater (2) at 298 K has been reported in four works:

Authors	Method	Salinity g salts/kg sln	10 ⁵ g(1)/100 g sln
Eganhouse and Calder (ref 1)	GLC	35	7.1
Schwarz (ref 2) u	v spectral	30	9.94
May et al. (ref 3)	HPLC	35	6.63
Aquan-Yuen et al. (ref 4) u	v spectral	28.6	8.3

At 298 K and a salinity of 35 g salts/kg sln the data of Eganhouse and Calder and of May *et al*. are in very good agreement. Therefore their mean,  $6.9 \times 10^{-5}$  g (1)/100 g sln is adopted as the recommended value for the solubility of phenanthrene at the indicated temperature and salinity. The value of Aquan-Yuen *et al*. appears consistent with the data discussed above and with the recommended value for the solubility of phenanthrene in pure water and is adopted at tentative. The value of Schwarz appears slightly high and is considered doubtful.

THE SOLUBILITY	OF	PHENANTHREN	E (1)	IN	SEAWATER	(2)
		RECOMMENDED	VALUE			

т/к	g salts/kg sln	10 ⁵ g(l)/100 g sln
298	35	6.9

REFERENCES

- Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.
- 2. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.
- 3. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.
- 4. Aquan-Yuen, M.; Mackay, D.; Shui, W.Y. J. Chem. Eng. Data <u>1979</u>, 24, 30-4.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Eganhouse, R.P.; Calder, J.A.
(2) Artificial seawater (ref. 1)	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25.0°C	M. Kleinschmidt and W. Shiu
Salinity: 35 g/kg sln	
EXPERIMENTAL VALUES:	
The solubility of phenanthrene in sea	water is reported to be 0.71 mg/kg
the corresponding mass percent and mo	
the compilers are 7.1 x $10^{-5}$ g(1)/100	g sln and 7.4 x $10^{-8}$ .
Graphical results for other salinitie	s are also reported.
	_
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium flask: 1-dm ³ Erlenmeyer	(1) analytical grade salt for
flask with ground glass stopper and sidearm tap at base plugged with	artificial seawater solution, reagent grade.
glass wool. The mixtures were agita-	Water: doubly distilled.
ted 12+ hr at 215 rpm on a New Bruns- wick gyrotary shaker; a 24 hr sta-	
tionary equilibrium period followed.	
Hydrocarbons were extracted with doubly-distilled hexane 3 times;	
concentrated by evaporation, with	
losses checked against an internal standard.	ESTIMATED ERROR:
Analysis: gas chromatography.	temperature: ± 0.5°C
	soly: ± 0.025 (95% confidence interval)
	REFERENCES:
	1. Lyman, J.; Fleming, R.H.; J. Mar. Res. <u>1940</u> , 3, 135.
1	

COMPONENTS :	ORIGINAL MEASUREMENTS:
	Schwarz, F.P.
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	
<pre>(2) Sodium chloride; NaCl; [7647-14-5]</pre>	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water; H ₂ O; [7732-18-5]	
ARIABLES:	PREPARED BY:
Cemperature: 11.1 - 31.8°C	W.Y. Shiu, D. Mackay
Salinity: 30 g(2)/kg sln	
XPERIMENTAL VALUES:	
Solubility of phenanthrene	in 0.5 mol(2)/L
$t/^{\circ}C$ 10 ⁶	nol(l)/L_sln
	. 88
1110	.2 .07
20.2 4	.51
	. 75 . 72
29.3 7	. 2
31.8 7	.9
$sln$ and $1.034 \times 10^{-7}$ .	ompilers are 9.94 x 10 ⁻⁵ g(l)/100 g
$sln$ and $1.034 \times 10^{-7}$ .	
	INFORMATION
AUXILIARY ETHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was	INFORMATION
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor-	INFORMATION SOURCE AND PURITY OF MATERIALS:
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of ohenanthrene was added to an air- ight 1X1 cm quartz fluorescence	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9%
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of obenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu-	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rp for at least 72 hr in a thermostated	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column.
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rp for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column.
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rp for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column.
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rp for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rp for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR:
AUXILIARY GETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpf for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author)
AUXILIARY AETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpf for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution and therefore provide an absolute	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author) Temperature ± 0.1°C (author) REFERENCES:
AUXILIARY AUXILIARY AETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpf for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author) Temperature ± 0.1°C (author) REFERENCES:
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AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluor- escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpf for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution and therefore provide an absolute solubility scale for the fluorescence	INFORMATION SOURCE AND PURITY OF MATERIALS: Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author) Temperature ± 0.1°C (author) REFERENCES:

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COMPONENTS :	ORIGINAL MEASUREMENTS:
	May, W.E.; Wasik, S.P.; Freeman,
(1) Phenanthrene; $C_{14}H_{10}$ ; [85-01-8]	D.H.
(2) Sodium Chloride; NaCl; [7647-14-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of phenanthrene in aquin terms of the Setschenow equation:	ueous sodium chloride is reported
$\log(S_{o}/S) = K_{S}C_{S}$	
where;	
S is the solubi	lity of (1) in water (mg/L)
U U	ity of (1) in saline solution $(mg/L)$
	_
5	enow constant (L/mol)
	tration of sodium chloride (mol/L)
evaluating the equation for S over the	he range of $C_{s}^{0-0.7 \text{ mol/L}}$ ,
$K_{\rm s} = 0.275$ with $S_{\rm o} = 1.002$ .	
The corresponding mass percent and ma	ole fraction $x_1$ , at salinity =
35 g(2)/kg sln calculated by the com	pilers are 6.63 x $10^{-5}$ g(1)/100 g sln
and 6.78 x $10^{-8}$ .	
Graphical data for other temperatures	s are also presented.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was	(1) greater than 97% pure.
prepared by pumping salt water through a "generation column" which	(2) reagent grade.
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium
saturated solution was extracted with an "extractor column" packed	permanganate-sodium hydroxide
with a superficially porous bonded	and passed through an XAD-2 column.
C ₁₈ stationary phase, then a water- acetonitrile solvent was passed	{
through for extraction. The extract was introduced into a	
liquid chromatograph and the concen-	ESTIMATED ERROR:
tration of (1) was measured with a UV detector.	temp $\pm 0.05^{\circ}C$ K_ $\pm 0.010$
	K ± 0.010 S ₀ ± 0.011
	REFERENCES :
	1

COMPONENTS:	ORIGINAL MEASU		
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Aquan-Yue Shiu, W.Y	n, M.; Mackay, I •	D.;
<pre>(2) Sodium chloride; NaCl;     [7647-14-5]</pre>	J. Chem.	Eng. Data <u>1979</u>	, 24, 30-4.
(3) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:	·	
One temperature: 25°C	M. Kleinschmidt and W. Shiu		
Salinity: 29-108 g(2)/kg sln			
EXPERIMENTAL VALUES:			
Solubility of phenanth	rene in aque	ous NaCl	
mol(2)/L sln g(2)/kg sln ^a mg	(1)/L sln	10 ⁵ mass%(1) ^a	$10^8 x_1^a$
0.50 28.6	0.85	8.3	8.6
1.00 56.2 1.50 82.6	0.67 0.48	6.4 4.5	6.8 4.9
2.00 108.2	0.33	3.1	3.3
AUXILIARY	INFORMATION		
· · · · · · · · · · · · · · · · · · ·		RITY OF MATERIALS:	
METHOD/APPARATUS/PROCEDURE: Saturated solutions were prepared	SOURCE AND PU	escence grade, f	rom
METHOD/APPARATUS/PROCEDURE: Saturated solutions were prepared by adding excess (1) to a pre- viously prepared salt solution.	SOURCE AND PU (1) fluore Eastma	escence grade, f an Kodak.	
METHOD/APPARATUS/PROCEDURE: Saturated solutions were prepared by adding excess (1) to a pre-	SOURCE AND PU (1) fluore Eastma	escence grade, f an Kodak. at grade, from F	
METHOD/APPARATUS/PROCEDURE: Saturated solutions were prepared by adding excess (1) to a pre- viously prepared salt solution. The resulting mixture was stirred for 24 hours and then allowed to settle for 48 hours. An aliquot was extracted with cyclohexane which was then analyzed spectro-	SOURCE AND PU (1) fluore Eastma (2) reager Scient	escence grade, f an Kodak. at grade, from F ific. OR:	
METHOD/APPARATUS/PROCEDURE: Saturated solutions were prepared by adding excess (1) to a pre- viously prepared salt solution. The resulting mixture was stirred for 24 hours and then allowed to settle for 48 hours. An aliquot was extracted with cyclohexane which was then analyzed spectro-	SOURCE AND PU (1) fluore Eastma (2) reager Scient ESTIMATED ERR temp ± 0.5	escence grade, f an Kodak. at grade, from F tific. OR: 5°C	
METHOD/APPARATUS/PROCEDURE: Saturated solutions were prepared by adding excess (1) to a pre- viously prepared salt solution. The resulting mixture was stirred for 24 hours and then allowed to settle for 48 hours. An aliquot was extracted with cyclohexane which was then analyzed spectro-	SOURCE AND PU (1) fluore Eastma (2) reager Scient	escence grade, f an Kodak. at grade, from F tific. OR: 5°C	
METHOD/APPARATUS/PROCEDURE: Saturated solutions were prepared by adding excess (1) to a pre- viously prepared salt solution. The resulting mixture was stirred for 24 hours and then allowed to settle for 48 hours. An aliquot was extracted with cyclohexane which was then analyzed spectro-	SOURCE AND PU (1) fluore Eastma (2) reager Scient ESTIMATED ERR temp ± 0.5 soly ± 3 n REFERENCES: 1. Weast Chemin Edition	escence grade, f an Kodak. at grade, from F tific. OR: 5°C	book of 59th

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) (E)-Stilbene; C ₁₄ H ₁₂ ; [103-30-3]	Andrews, L.J.; Keefer, R.M.
(2) Water; $H_2^{0}$ ; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of (E)-stilbene in wat to be 2.9 x $10^{-5}$ g(1)/100 g sln.	er at 25°C was reported
The corresponding mole fraction, $x_1$ , is 2 x 10 ⁻⁸ .	calculated by the compilers
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
2 minutume of (1) and (2) upp	(1) from the State University of
A mixture of (1) and (2) was rotated for twenty hours in a	Iowa;
constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous	m.p. 120-121°C;
phase was withdrawn and extracted with a measured volume of hexane	(2) not specified.
(10-50 mL) by shaking in a glass-	
stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase	
was measured against a hexane blank on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:
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COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) 1,4-Dicyclopentylbutane; C ₁₄ H ₂₆ ; [2980-70-3]		Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]		Khim. Technol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:		PREPARED BY:
Temperature: 10-30°C		A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:		
Solubility (	of Water in 1	1,4-Dicyclopentylbutane
<u>t/°C</u>	g(2)/100 g s	$ln \qquad 10^3 x_2 (compiler)$
10 20 30	0.0088 0.0139 0.0241	0.94 1.50 2.59
	AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:
Component (1) was introduction thermostatted flask and a for 5 hr. with (2). Next hydride was added and the hydrogen volume measured the concentration of (2) evaluated.	saturated t, calcium e evolving and hence	<ul><li>(1) Not specified.</li><li>(2) Not specified.</li></ul>
		ESTIMATED ERROR:
		Not specified.
		REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

Quantitative solubility data for the tetradecane (1) - water (2) system have been reported in the publications listed in Table 1.

## TABLE 1: Quantitative Solubility Studies ofthe Tetradecane (1) - Water (2) System

Reference	Т /К	Solubility	Method
Schatzberg (ref 1)	313	(2) in (1)	Karl Fischer
Franks (ref 2)	298	(1) in (2)	GLC
Sutton and Calder (ref 3)	298	(1) in (2)	GLC
Mackay et al. (ref 4)	_ a	(1) in (2)	GLC

a Not specified but probably close to 298 K.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

### 1. SOLUBILITY OF TETRADECANE (1) IN WATER (2)

The solubility of tetradecane in water has been reported only at 298K (Table 1). Unfortunately, the results are in very poor agreement (Table 2). Furthermore, all the reported values are very much higher than the value of  $\sim 3 \times 10^{-8}$  g(1)/100 g sln which is predicted by extrapolation of the lower hydrocarbon homologue solubilities. Thus, the values given in Table 2 must be regarded very sceptically and no "Best" value has been calculated.

	<u>TAB</u>	LE 2: Reported Solubility Values of Tetradecane (1) in Water (2)
	Т / К	Reported solubility values ^{$\alpha$} 10 ⁷ g(1)/100 g sln
	298	6.94 (ref 2), 2.2 (ref 3), 25.9 ^b (ref 4)
	All values may be uncertainties in	high. "Best" values not determined because of data, see text.
2	Assumed to be at	298K for the purpose of comparison.

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(continued next page)

COMPONENTS:	EVALUATOR:
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN TETRADECANE

As only the datum of Schatzberg at 313K is available no Critical Evaluation is possible. However, it may be noted that the data of Schatzberg in well characterized systems are generally reliable. The interested user is referred to the appropriate Data Sheet for the experimental value.

### REFERENCES

- 1. Schatzberg, P. J. Phys. Chem. <u>1963</u>, 67, 776-9.
- 2. Franks, F. Nature (London) <u>1966</u>, 210, 87-8.
- 3. Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u>, 8, 654-7.
- Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. <u>1975</u>, 573, 251-8.

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ORIGINAL MEASUREMENTS:
Schatzberg, P.
J. Phys. Chem. <u>1963</u> , 67, 776-9.
PREPARED BY:
M.C. Haulait-Pirson
<u> </u>
he at 40°C was reported to be mole fraction, $x_2$ , of 1.26 x 10 ⁻⁵ .
INFORMATION
<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co.; pure grade; 99+ mole %; passed repeatedly through a column of silica gel until no absorp- tion occurred in the 220 to 340 nm spectral range. (2) distilled and deionized. ESTIMATED ERROR: temp. ± 0.02°C soly. 0-2% (deviations from the mean) REFERENCES:</pre>

	OPTOTWAL MELCUPPLETING
Components :	ORIGINAL MEASUREMENTS:
(1) Tetradecane; H ₁₄ H ₃₀ ; [629-59-4]	Franks, F.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) <u>1966</u> , 210, 87-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of tetradecane in wate	r at 25°C was reported to be
in mole fraction $x_1 = 6.3 \times 10^{-10}$ .	
The corresponding mass percent calcul	ated by the compiler is
$6.94 \times 10^{-7} g(1)/100 g sln.$	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	
The analysis was performed by gas liquid chromatography. After	<pre>(1) Fluka; purum grade; purity &gt; 97% (chromatographic</pre>
equilibrating the (1)/(2) mixtures	analysis).
in a thermostat, up to 0.5 mL of the aqueous phase was injected into the	(2) not specified.
fractionator fitted to the chroma- tographic column, and (2) was	
removed by "Drierite". The (1) concentrations were obtained from	
the peak areas, after initial	
calibrations.	ESTIMATED ERROR:
1	soly. ± 12%
	REFERENCES :

	ORIGINAL MEASUREMENTS:	
Components :	ORIGINAL MEASUREMENTS:	
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4]	Sutton, C.; Calder, J.A.	
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.	
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VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of tetradecane in water at 25°C was reported to be 2.2 x $10^{-7}$ g(1)/100 g(2) corresponding to a mole fraction $x_1$ , of 2 x $10^{-10}$ .		
	THEODIARTON	
	INFORMATION	
METHOD/APPARATUS/PROCEDURE: 175 mg (1) were equilibrated with 700 mL (2) in closed flasks by sha- king on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane con- taining an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization de- tectors.	SOURCE AND PURITY OF MATERIALS: (1) Analabs Inc., 99+%. (2) doubly distilled. ESTIMATED ERROR: temp. ± 0.1°C soly. ± 16% REFERENCES:	

والمحمي والمحمد المنافعة ومعادلة بالمحمد والمنافع والمنتج والمنتج ومحمد والمحمد والمحمد والمحمد والمحمد والم		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4]	Mackay, D.; Shiu, W.J.; Wolkoff, A.W.	
(2) Water; H ₂ O; [7732-18-5]	"Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. <u>1975</u> , 573, 251-8.	
VARIABLES:	PREPARED BY:	
not specified	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The authors reported a value of 0.0259 mg(1)dm ⁻³ sln for the solubility of tetradecane in water. With the assumption of a solution density of 1.00 g cm ⁻³ the corresponding mass percent, calculated by the compiler, is 2.59 x $10^{-6}$ g(1)/100 g sln and the corresponding mole fraction, $x_1$ , is 2.4 x $10^{-9}$ .		
AUXILIARY	INFORMATION	
ME THOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS;	
(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equili- brations it is possible to calculate the amount of (1) in the original sample.	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>	

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COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4]	Sutton, C.; Calder, J.A.	
(2) Seawater	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C One salinity: 35 g salts/kg sln	P.A. Meyers and D. Shaw	
EXPERIMENTAL VALUES:		
The solubility of tetradecane in seawater was reported to be 1.7 x $10^{-7}$ g(1)/100 g sln and $x_1 = 1.5 \times 10^{-10}$ .		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The com- ponents were equilibrated by gentle shaking for 12 hrs at $25.0 \pm 0.1^{\circ}$ C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 µm membrane filters to remove any hydrocarbon droplets. The filtrate was extrac- ted three times with hexane and ana- lyzed by gas chromatography.	<pre>Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</pre>	
	ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.	
	REFERENCES:	

COMPONENTS :	EVALUATOR:
<pre>(1) 2-Methylanthracene; C₁₅H₁₂; [613-12-7] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

Quantitative solubility data for 2-methylanthracene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 2-methylanthracene.

## TABLE 1: Quantitative Solubility Studies of2-Methylanthracene (1) in Water (2)

Reference	Т /К	Method
Mackay and Shiu (ref 1)	298	spectofluorometric
May <i>et al</i> . (ref 2)	279-304	chromatographic

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

At 298K, the only temperature at which comparison is possible, the datum of Mackay and Shiu (ref 1) is in only fair agreement with that of May *et al.* (ref 2). Thus all the available data, which are summarized in Table 2, must be regarded as very tentative.

## TABLE 2: Tentative Solubility Values of 2-Methylanthracene (1) in Water (2)

т /к	Solubility values		-
	Reported values ^{$a$}	"Best values	$(\pm \sigma_n)^b$
	10 ⁶ g(1)/100 g sln	10 ⁶ g(1) g sln	$10^9 x$
278	0.64* (ref 2)	0.6	0.6
283	0.89* (ref 2)	0.9	0.8
293	1.60* (ref 2)	1.6	1.5
298	3.9 (ref 1), 2.16* (ref 2)	3.0 ± 0.9	2.8
303	2.93 (ref 2)	3.0	2.8

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.

b Obtained by averaging where appropriate;  $\boldsymbol{\sigma}_n$  has no statistical significance.

REFERENCES

1. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

2. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

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COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) 2-Methylanthracene; C ₁₅ H ₁₂ ;	Mackay, D.; Shiu, W.Y.	
[613-12-7]	J. Chem. Eng. Data <u>1977</u> , 22,	
(2) Water; H ₂ O; [7732-18-5]	399-402.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of 2-methylanthracene in water at 25°C was reported to be 0.039 mg(1) dm ⁻³ sln and $x_1 = 3.67 \times 10^{-9}$ . The corresponding mass percent calculated by the compiler is 3.9 x 10 ⁻⁶ g(1)/100 g sln.		
	INFORMATION	
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.</li> <li>(2) doubly distilled.</li> </ul>	
	<pre>soly. ± 0.004 mg(1) dm⁻³ sln (maximum deviation from several determinations). REFERENCES:</pre>	

	• · · · · · · · · · · · · · · · · · · ·	430
COMPONENTS :	ORIGINAL MEASUREMENTS:	
<pre>(1) 2-Methylanthracene; C₁₅H₁₂; [613-12-7]</pre>	May, W.E.; Wasik, S.P. Angl. Chem. 1978. 50	
(2) Water; H ₂ O; [7732-18-5]	Anal. Chem. <u>1978</u> , 50, 175-9 and 997-1000.	
VARIABLES:	PREPARED BY:	
Temperature: 6.3-31.1°C	A. Maczynski	
EXPERIMENTAL VALUES:	I	<u> </u>
Solubility of 2-methy	lanthracene in water	
t/°C μg(1)/kg(2)	10 ⁶ g(l)/100 g sln (compiler)	$10^9 x_1$ (compiler)
6.3 7.06 ± 0.18	0.706	0.661
9.1 8.48 ± 0.09	0.848	0.794
10.8 9.43 ± 0.37	0.943	0.883
13.9 11.1 ± 0.3	1.11	1.04
18.3 14.5 ± 0.1	1.45	1.36
23.1 19.1 ± 0.6	1.91	1.79
25.0 21.3 ± 0.3	2.13	1.99
27.0 24.2 ± 0.1	2.42	2.27
31.1 32.1 ± 0.3	3.21	3.01
AUXILIARY	INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERI	IALS:
The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a	<ul> <li>(1) commercial production</li> <li>than 3% impurities</li> <li>(2) distilled over KM</li> </ul>	S.
column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the coupled column liquid chromato-	and passed through packed with XAD-2 Hass, Philadelphia	h a column (Rohm and
graphic process that has been	ESTIMATED ERROR:	
described in ref 1.	temp. ± 0.05°C soly. stand. dev. see	above
	REFERENCES:	<u> </u>
	1. May, W.; Chesler, S Gump, B.; Hertz, H Dyszel, S. J. Chro 1975, 13, 535.	.; Enagonio, D.

COMPONENTS :	ORIGINAL MEASUREMENTS:		
<pre>(1) 2-Methylanthracene; C₁₅H₁₂; [613-12-7]</pre>	May, W.E.; Wasik, S.P.; Freeman D.H.		
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997 <b>-</b> 1000.		
(3) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
One temperature: 25°C			
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay		
EXPERIMENTAL VALUES:			
The solubility of 2-methylanthracene	in aqueous sodium chloride is		
reported in terms of the Setschenow e	equation:		
$\log(S_{O}/S) = K_{S}C_{S}$			
where;			
S is the solubility of	S is the solubility of (1) in water (mg/L)		
, and a second s			
S is the solubility of (1) in saline solution $(mg/L)$			
$K_{s}$ is the Setschenow constant (L/mol)			
$C_{s}$ in the concentration of sodium chloride (mol/L)			
evaluating the equation for S over th	te range of $C_{s}$ 0-0.7 mol/L,		
$K_{\rm s} = 0.336$ with $S_{\rm o} = 0.0213$ .			
The corresponding mass percent and mo	le fraction $x_1$ , at salinity =		
35 g(2)/kg sln calculated by the comp	pilers are $1.29 \times 10^{-6} g(1)/100 g sln$		
and $1.24 \times 10^{-9}$ .			
AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A saturated solution of (1) was prepared by pumping salt water	(1) greater than 97% pure.		
through a "generation column" which was packed with glass beads coated	(2) reagent grade.		
with 1% by weight of (1). The saturated solution was extracted	(3) distilled from potassium permanganate-sodium hydroxide		

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was prepared by pumping salt water	(1) greater than 97% pure.
through a "generation column" which was packed with glass beads coated	(2) reagent grade.
with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C ₁₈ stationary phase, then a water- acetonitrile solvent was passed through for extraction. The	(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.
extract was introduced into a	ESTIMATED ERROR:
liquid chromatograph and the concen- tration of (1) was measured with a	temp $\pm 0.05$ °C
UV detector.	$K_{s} \pm 0.006$
	s _o ± 0.003
	REFERENCES :
	I I I I I I I I I I I I I I I I I I I

CONTRACTION OF A	ORIGINAL MEASUREMENTS:	
COMPONENTS:	Mackay, D.; Shiu, W.Y.	
<pre>(1) 9-Methylanthracene; C₁₅H₁₂;</pre>		
[779-02-2]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
•		
EXPERIMENTAL VALUES:		
The solubility of 9-methylanthracene in water at 25°C was reported to be 0.26l mg(1) dm ⁻³ sln and $x_1 = 2.44 \times 10^{-8}$ . The corresponding mass percent calculated by the compiler is 2.6l x 10 ⁻⁵ g(1)/100 g sln.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.002 mg(1) dm⁻³ sln (maximum deviation from several determinations). REFERENCES:</pre>	

		ORIGINAL MEASUREMENTS:		
(1) 1-Methylphena	inthrene; C ₁₅ H ₁₂ ;	May, W.E.; Wasik, S.P.	; Freeman, D.H.	
[832-69-6] (2) Water; H ₂ O; [	7732-18-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.	175-9 and	
-				
VARIABLES:	<u></u>	PREPARED BY:		
Temperature: 6.6-29.9°C		A. Maczynski		
EXPERIMENTAL VALUES:	· · · · · · · · · · · · · · · · · · ·	I		
Sc	olubility of 1-methyl	Iphenanthrene in water		
t/°C	μg(l)/kg(2)	10 ⁵ g(1)/100 g sln (compiler)	10 ⁸ x1 (compiler)	
6.6	95.2 ± 0.2	0.952	0.892	
8.9	114.0 ± 4.0	1.14	1.07	
14.0	147.0 ± 1.0	1.47	1.38	
19.2	193.0 ± 1.0	1.93	1.81	
24.1	255.0 ± 5.0	2.55	2.39	
25.0	269.0 ± 3.0	2.69	2.69	
26.9	304.0 ± 1.0	3.04	2.85	
29.9	355.0 ± 2.0	3.55	3.32	
	AUXILIARY	INFORMATION		
ME THOD / APPARATUS / PROC		INFORMATION SOURCE AND PURITY OF MATERI		
The dynamic coupl chromatography (I based on generati tions by pumping column packed wit have been coated (1) (generator co centration of (1) of the generator sured by a modifi	EDURE: Led column liquid DCCLC) method was ing saturated solu- water through a th glass beads that with the component olumn). The con- in the effluent column was mea- ication of the		t; less 5. nO ₄ and NaOH n a column (Rohm and	
The dynamic coupl chromatography (I based on generati tions by pumping column packed wit have been coated (1) (generator co centration of (1) of the generator sured by a modifi coupled column 1	EDURE: Led column liquid DCCLC) method was ing saturated solu- water through a th glass beads that with the component olumn). The con- in the effluent column was mea- ication of the iquid chromato-	<ul> <li>SOURCE AND PURITY OF MATERI</li> <li>(1) commercial product than 3% impurities</li> <li>(2) distilled over KMr and passed through packed with XAD-2 Hass, Philadelphia</li> </ul>	t; less 5. nO ₄ and NaOH n a column (Rohm and	
The dynamic coupl chromatography (I based on generati tions by pumping column packed wit have been coated (1) (generator co centration of (1) of the generator sured by a modifi coupled column 1	EDURE: Led column liquid DCCLC) method was ing saturated solu- water through a th glass beads that with the component olumn). The con- in the effluent column was mea- ication of the iquid chromato- that has been de-	<pre>SOURCE AND PURITY OF MATERI (1) commercial product than 3% impurities (2) distilled over KMr and passed through packed with XAD-2 Hass, Philadelphia ESTIMATED ERROR:</pre>	t; less 5. nO ₄ and NaOH n a column (Rohm and	
The dynamic coupl chromatography (I based on generati tions by pumping column packed wit have been coated (1) (generator co centration of (1) of the generator sured by a modifi coupled column 1i graphic process t	EDURE: Led column liquid DCCLC) method was ing saturated solu- water through a th glass beads that with the component olumn). The con- in the effluent column was mea- ication of the iquid chromato- that has been de-	<ul> <li>SOURCE AND PURITY OF MATERI</li> <li>(1) commercial product than 3% impurities</li> <li>(2) distilled over KMr and passed through packed with XAD-2 Hass, Philadelphia</li> </ul>	t; less s. hO ₄ and NaOH h a column (Rohm and a, Pa).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Methylphenanthrene; C₁₅H₁₂; [832-69-9]</pre>	May, W.E.; Wasik, S.P.; Freeman, D.H.
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of l-methylphenanthre	ne in aqueous sodium chloride is
reported in terms of the Setschenow	equation:
$log(S_0/S) = K_SC_S$	
where;	
S is the solubility	of (l) in water (mg/L)
S is the solubility o	f (l) in saline solution (mg/L)
K _c is the Setschenow	
5	on of sodium chloride (mol/L)
5	
evaluating the equation for S over t	s range of C _s 0-0.7 mol/L,
$K_{\rm s} = 0.211$ with $S_{\rm o} = 0.269$ .	
The corresponding mass percent and m	ole fraction $x_1$ , at salinity =
	pilers are $1.95 \times 10^{-5} g(1)/100 g sln$
and $1.87 \times 10^{-8}$ .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was prepared by pumping salt water	(1) greater than 97% pure.
through a "generation column" which was packed with glass beads coated	(2) reagent grade.
with 1% by weight of (1). The	(3) distilled from potassium
saturated solution was extracted with an "extractor column" packed	permanganate-sodium hydroxide and passed through an XAD-2
with a superficially porous bonded $C_{10}$ stationary phase, then a water-	column.
acetonitrile solvent was passed through for extraction. The	
extract was introduced into a liquid chromatograph and the concen-	ESTIMATED ERROR:
tration of (1) was measured with a	temp ± 0.05°C
UV detector.	$     K \pm 0.018     S^{S} \pm 0.003   $
	REFERENCES:
	ļ

COMPONENTS: (1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. June 1986.

### CRITICAL EVALUATION:

Quantitative solubility data for fluoranthene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in fluoranthene.

# TABLE 1. Quantitative Solubility Studies ofFluoranthene (1) in Water (2)

Reference	т / К	Method
Davis et al. (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May et al. (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. They are also summarized in Table 2. The values at 298 K are in reasonable agreement given the low solubility and the average value is Recommended. The remaining data are regarded as Tentative only.

TABLE	2.	Recon	mended	(R)	and	Tenta	ative	
Solubility	Valu	es of	Fluorar	ther	1e (1	<u>) in</u>	Water	(2)

Т /К	Solu	bility values	
	Reported values 10 ⁵ g(1)/100 g sln	"Best" values ( 10 ⁵ g(1)/100 g sln 1	
298	2.65 (ref 2), 2.6 (ref 3), 2.06 (ref 4)	2.4 ± 0.3 (R) 2	2.1 ( <i>R</i> )
300	2.40 (ref 1)	2.4	2.1
302	2.64 (ref 4)	2.6	2.3

a Obtained by averaging where appropriate;  $\sigma_{\rm n}$  has no statistical significance.

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402.
- 4. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. 1978, 50, 997-1000.

	ORIGINAL MEASUREMENTS:
(1) Elucranthene: $C$ H : [206-44-0]	Davis, W.W.; Krahl, M.E.;
16 10 1	Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of flu	oranthene in water
t/°C	$10^4$ g(1) L ⁻¹ (2)
27	2.40 ± 0.20
	2.25 ± 0.20
	2.40 ± 0.20
AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
	1
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University;    m.p. range ll0.0-ll0.7°C;    (cf. ref 2). (2) dust-free. ESTIMATED ERROR:</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University;    m.p. range 110.0-110.7°C;    (cf. ref 2). (2) dust-free.</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University;    m.p. range 110.0-110.7°C;    (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C</pre>

COMPONENTS: (1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) Water; H₂O; [7732-18-5] VARIABLES: ORIGINAL MEASUREMENTS: Klevens, H.B. J. Phys. Chem. <u>1950</u>, 54, 283-98.

Temperature: 25°C

### EXPERIMENTAL VALUES:

The solubility of fluoranthene in water at 25°C was reported to be 2.65 x  $10^{-4}$  g(1) L⁻¹ and 1.32 x  $10^{-6}$  mole/L⁻¹. Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 2.65 x  $10^{-5}$  g(1)/100 g sln and 2.37 x  $10^{-8}$ .

M.C. Haulait-Pirson

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of fluoranthene in wat to be 0.26 mg(1) dm ⁻³ sln and $x_1 = 2$ .	
The corresponding mass percent calcul is 2.6 x $10^{-5}$ g(1)/100 g sln.	ated by the compiler
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	<ul> <li>(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.</li> </ul>
Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory	(2) doubly distilled.
funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. $\pm$ 0.002 mg(1) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES:
<u></u>	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]	May, W.E.; Wasik, S.P.; Free	
(2) Water; H ₂ O; [7732-18-5]	Anal. Chem. <u>1978</u> , 50, 997-1	000.
VARIABLES:	PREPARED BY:	
Temperature: 25 and 29°C	A. Maczynski	
EXPERIMENTAL VALUES:	I	
Solubility of fluo	ranthene in water	
t/°C mg(1)/kg(2)		0 ⁸ x1 piler)
25 0.206	2.06 1	.83
29 0.264	2.64 2	.35
AUXILIARY	INFORMATION	
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:	
METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the coupled column liquid chromato-	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) commercial product; less than 3% impurities.</li> <li>(2) distilled over KMnO₄ and and passed through a col packed with XAD-2 (Rohm Hass, Philadelphia, Pa).</li> </ul>	NaOH umn and
METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) commercial product; less than 3% impurities.</li> <li>(2) distilled over KMnO₄ and and passed through a col packed with XAD-2 (Rohm Hass, Philadelphia, Pa).</li> <li>ESTIMATED ERROR:</li> </ul>	NaOH umn and
METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the coupled column liquid chromato- graphic process that has been	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) commercial product; less than 3% impurities.</li> <li>(2) distilled over KMnO₄ and and passed through a col packed with XAD-2 (Rohm Hass, Philadelphia, Pa).</li> </ul>	NaOH umn and
METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the coupled column liquid chromato- graphic process that has been	<pre>SOURCE AND PURITY OF MATERIALS: (1) commercial product; less than 3% impurities. (2) distilled over KMnO₄ and and passed through a col packed with XAD-2 (Rohm Hass, Philadelphia, Pa). ESTIMATED ERROR: temp. ± 0.05°C soly. ± 0.002 mg(1)/kg(2)</pre>	m, S.;

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]	May, W.E.; Wasik, S.P.; Freeman, D.H.
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of fluoranthene in aq	ueous sodium chloride is
reported in terms of the Setschenow	equation:
log(S _o /S) = K _s C _s	
where;	
S is the solubility	of (l) in water (mg/L)
e e e e e e e e e e e e e e e e e e e	f (l) in saline solution (mg/L)
K is the Setschenow	
5	
5	on of sodium chloride (mol/L)
evaluating the equation for S over the	he range of C 0-0.7 mol/L, s
$K_{\rm s} = 0.339$ with $S_{\rm o} = 0.206$ .	
The corresponding mass percent and ma	ole fraction $x_{1}$ , at salinity =
35 g(2)/kg sln calculated by the com	-
sin and 1.14 x $10^{-8}$ .	pricis die 1.24 g x 10 g(1)/100 g
sin and 1.14 x 10 .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was prepared by pumping salt water	(1) greater than 97% pure.
through a "generation column" which was packed with glass beads coated	(2) reagent grade.
with 1% by weight of (1). The	(3) distilled from potassium
saturated solution was extracted with an "extractor column" packed	permanganate-sodium hydroxide and passed through an XAD-2
with a superficially porous bonded C ₁₈ stationary phase, then a water-	column.
acetonitrile solvent was passed through for extraction. The	
extract was introduced into a	
liquid chromatograph and the concen- tration of (1) was measured with a	temp ± 0.05°C
UV detector.	$     K_{o} \stackrel{\pm}{=} 0.010     S_{o} \stackrel{\pm}{=} 0.002   $
	REFERENCES:
L	

COMPONENTS:	EVALUATOR:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

Quantitative solubility data for pyrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in pyrene.

TABLE 1.	Quantitative Solubility Studies	of
	Pyrene (1) in Water (2)	

Reference	Т / К	Method nephelometric	
Davis et al. (ref 1)	300		
Klevens (ref 2)	298	spectrophotometric	
Wauchope and Getzen (ref 3)	273-348	spectrophotometric	
Mackay and Shiu (ref 4)	298	spectrofluorometric	
Schwarz (ref 5)	285-304	spectrofluorometric	
May et al. (ref 6)	298-302	chromatographic	
Rossi and Thomas (ref 7)	298	GLC, spectrophotometric	

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. At 298 K the values of Mackay and Shiu (ref 4), Schwarz (ref 5), May *et al.* (ref 6) and Rossi and Thomas (ref 7) are in excellent agreement and their average is Recommended. The values of Wauchope and Getzen (ref 3) and especially Klevens (ref 2) are signifigantly higher  $(>3\sigma_n)$  than the other studies and are thus rejected. At 303 K the values of Wauchope and Getzen (ref 3) are in good agreement with those of Schwarz (ref 5) and May *et al.* (ref 6). At other temperatures the data are mainly those of Wauchope and Getzen and must therefore be regarded as Tentative.

With the exception of the rejected values noted above and the 300 K datum of Davis *et al*. (ref 1) which is omitted for representational convenience, all the available data are summarized in Table 2. Selected data are also plotted in Figure 1.

COMPONENTS:	EVALUATOR:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

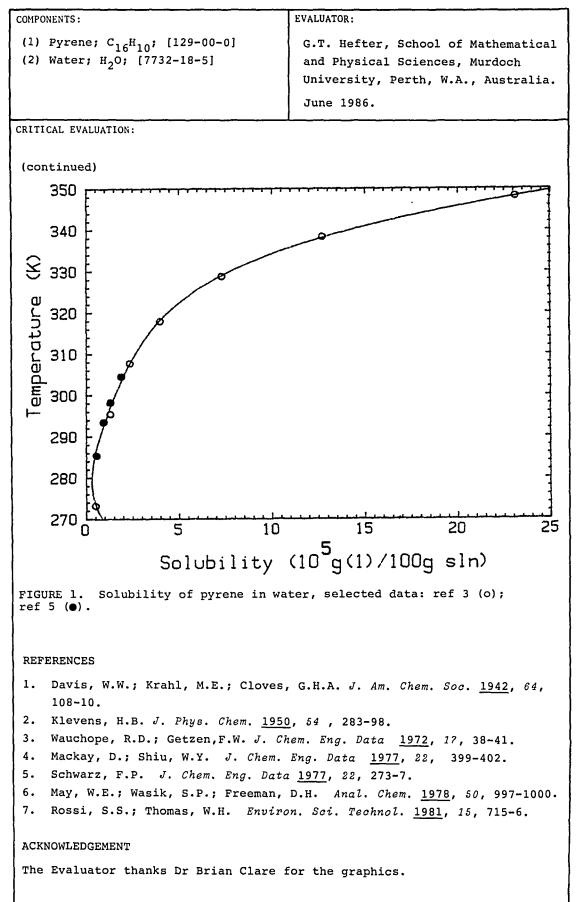
(continued)

## TABLE 2. Recommended (R) and Tentative Solubility Values of Pyrene (1) in Water (2)

Т/К	Solubilit	Solubility values			
Reported va	Reported values ^a	"Best" value	"Best" values $(\pm \sigma_n)^b$		
	10 ⁵ g(1)/100 g sln	10 ⁵ g(1)/100 g sln	$10^8 x_1$		
273	0.49 (ref 3)	0.5	0.4		
293	0.91* (ref 5)	0.9	0.8		
298	1.35 (ref 4), 1.295 (ref 5),	$1.32 \pm 0.02(R)$	1.17(R)		
	1.32 (ref 6), 1.3 (ref 7)				
303	1.80* (ref 3), 1.76* (ref 5),	1.75 ± 0.04(R)	1.56(R)		
	1.70* (ref 6)				
313	3.30* (ref 3)	3	3		
323	5.32 (ref 3)	5	4		
333	9.4* (ref 3)	9	8		
343	16.9 (ref 3)	17	15		
348	23.1 (ref 3)	23	20		

a Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the authors' original data.

b Obtained by averaging where appropriate;  $\sigma_{\rm n}$  has no statistical significance.



2040010175 ·	OPTCTNAT WEACHIDEVENING		
COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.		
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. 1942, 64,		
	108-10.		
VARIABLES:	PREPARED BY:		
	M.C. Haulait-Pirson		
One temperature: 27°C			
EXPERIMENTAL VALUES:			
	umono in votor		
Solubility of p	$10^4 \text{ g(1) } \text{L}^{-1} \text{ (2)}$		
<i>t/°C</i>			
27	1.60 ± 0,10		
	1.65 ± 0.05		
The best value recommended by the aut	hors is $1.65 \times 10^{-4}$ g(1) L ⁻¹ (2).		
Assuming that 1.00 L sln = 1.00 kg	sln the corresponding mass percent		
and mole fraction, $x_1$ , calculated by			
100 g sln and 1.45 $\times 10^{-8}$ .			
AUXILIARY	INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
The method consisted of preparing	(1) prepared at Harvard University;		
serial dilutions of a suspension of (1) in (2) and determining	<pre>m.p. range 149.6-150.5°C; (cf. ref 2).</pre>		
nephelometrically the amount of			
(1) per unit volume beyond which further dilution caused no reduc-	(2) dust-free.		
tion in light scattering, which remained equal to that of pure (2).			
A Bausch and Lomb Dubosque colori-			
meter model 100-mm was employed. Many details are reported in ref 1.			
	ESTIMATED ERROR:		
	temp. ± 3°C soly. see above		
	-		
	REFERENCES :		
	1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64,		
	101.		
	2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc.		
	<u>1940</u> , <i>62</i> , 3086.		

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Pyrene; C₁₆H₁₀; [129-00-0] Klevens, H.B. (2) Water; H₂O; [7732-18-5] J. Phys. Chem. 1950, 54, 283-98. VARIABLES: PREPARED BY: M.C. Haulait-Pirson Temperature: 25°C EXPERIMENTAL VALUES: The solubility of pyrene in water at 25°C was reported to be  $1.75 \times 10^{-4} g(1) L^{-1} sln and 7.7 \times 10^{-7} mol(1) L^{-1} sln.$ Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 1.75 x  $10^{-5}$  g(1)/ 100 g sln and 1.39  $\times 10^{-8}$ . AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The solubility of (1) in (2) was (1) not specified. determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were (2) not specified. removed and concentrations determined by spectra. ESTIMATED ERROR: not specified. **REFERENCES:** 

COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Wauchope, R.D.; Getzen, F.W.		
10 10			
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.		
VARIABLES :	PREPARED BY:		
Temperature: 0-75°C	A. Maczynski		
EXPERIMENTAL VALUES:			
EAFERIPENTAL VALUED.			
Solubility of pyre	ne in water		
t/°C mg(1)/kg(2) smoothed w	$\frac{1}{10^5}$ g(1)/100 g sln $10^8 x_1$		
t/°C smoothed w experiment(std_dev			
0.0 0.049(0	.001) 0.49 0.44		
22.2 0.129, 0.128, 0.124 0.130 25.0 0.148 (0	1.30 1.15		
34.5 0.228, 0.235 0.235	2.35 2.09		
44.7 0.397, 0.395, 0.405 0.399	3.99 3.55 .004) 5.32 4.74		
50.0 0.532(0 50.1 0.558, 0.576, 0.556 0.534	.004) 5.32 4.74 5.34 4.75		
55.6 0.75, 0.75, 0.77 0.73	7.3 6.5		
56.0         0.74         0.74           60.7         0.96, 0.95, 0.90         0.97	7.4 6.6 9.7 8.6		
65.2 1.27, 1.29 1.27	12.7 11.3		
71.9         1.83,         1.86,         1.89         1.90           74.7         2.21         2.26	19.0 16.9 22.6 20.1		
75.0 2.31(0.			
AUXILIAR	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Approximately 20 g of (1) was placed in each of three 250-mL glass-	(1) Baker reagent; recrystallized three times from ether;		
stoppered flasks with (2). The	vacuum-sublimed twice;		
flasks were suspended in an open water bath and shaken gently from	purity not specified.		
one to three weeks between measure-	(2) distilled and deionized.		
ments. Samples of the replicate wer extracted with cyclohexane. In all	e		
cases, spectra taken of second			
extracts or of the aqueous layer after extraction indicated complete			
extraction.	ESTIMATED ERROR:		
Standard solutions were prepared either by direct weighing using a	temp. ± 0.5°C		
Cahn electrobalance, or by weighing	soly. see experimental values		
0.1-0.2 g of samples followed by serial dilution in calibrated glass-	above		
ware.			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of pyrene in water at to be 0.135 mg(1) dm ⁻³ sln and $x_1 = 1$	
The corresponding mass percent calcul	lated by the compiler
is 0.0000135 g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories,
flask for 24 hrs. and subsequently	commercial highest grade;
settled at 25°C for at least 48 hrs. Then the saturated solution was	used as received.
decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. $\pm$ 0.005 mg(l) dm ⁻³ sln
In the paper.	(maximum deviation from several determinations).
	REFERENCES :

COMPONENTS	·····	ORIGINAL MEASUREMENTS:	
COMPONENTS :		ORIGINAL MEASUREMENIS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [	129-00-0]	Schwarz, F.P.	
(2) Water; H ₂ O; [7732	-18-5]	J. Chem. Eng. Data 19	<u>77</u> , 22, 273-7.
2			
VARIABLES:		PREPARED BY:	
Temperature: 12.2-31.	3°C	A. Maczynski	
EXPERIMENTAL VALUES:			
	Solubility of p	pyrene in water	
t/°C 10 ⁷	$mol(1) L^{-1}$	10 ⁶ g(1)/100 g sln	$10^{9}x_{1}$
		(compiler)	(compiler)
12.2	2.70 ± 0.03	5.46	4.86
15.5	3.39 ± 0.03	6.86	6.11
17.4	3.91 ± 0.05	7.91	7.04
	$4.57 \pm 0.04$	9.25	8.23
	5.78 ± 0.06	11.69	10.41
	5.82 ± 0.03	11.77	10.48
	6.40 ± 0.05	12.95	11.53
	7.13 ± 0.07	14.42	12.84
	7.18 ± 0.04 8.09 ± 0.08	14.53 16.37	12.93 16.90
31.3	$9.3 \pm 0.1$	18.81	16.75
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE	:	SOURCE AND PURITY OF MATERI	ALS:
Two methods were used	l.	(1) source not specif:	
At 25°C the solubilit	v of (1) in (2)	than 99 mole%, by glc;	
was determined from U	W absorption		
measurements and was standard at other tem		(2) distilled over KMM and passed through	
At other temperatures		column.	L
spectrofluorimetry me			
The sealed fluorescen	ce cells	1	
contained 5 mL of the solution and an exces	aqueous s of (1) were		
contained 5 mL of the	aqueous s of (1) were in a water	ESTIMATED ERROR:	
contained 5 mL of the solution and an exces rotated at least 72 h	aqueous s of (1) were in a water uickly wiped	temp. ± 0.1°C	······
contained 5 mL of the solution and an excess rotated at least 72 h bath, then removed, o	aqueous s of (1) were in a water uickly wiped		
contained 5 mL of the solution and an excess rotated at least 72 h bath, then removed, o	aqueous s of (1) were in a water uickly wiped	temp. ± 0.1°C	
contained 5 mL of the solution and an excess rotated at least 72 h bath, then removed, o	aqueous s of (1) were in a water uickly wiped	temp. ± 0.1°C soly. see above	
contained 5 mL of the solution and an excess rotated at least 72 h bath, then removed, o	aqueous s of (1) were in a water uickly wiped	temp. ± 0.1°C soly. see above	
contained 5 mL of the solution and an excess rotated at least 72 h bath, then removed, o	aqueous s of (1) were in a water uickly wiped	temp. ± 0.1°C soly. see above	

.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	May, W.E.; Wasik, S.P.; Freeman, D.H.
(2) Water; H ₂ O; [7732-18-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.
VARIABLES:	PREPARED BY:
Temperature: 25 and 29°C	A. Maczynski
EXPERIMENTAL VALUES:	L
EAFERINENIAL VALUES.	
Solubility of p	pyrene in water
t/°C mg(1)/kg(2)	$10^5 g(1)/100 g sln 10^8 x_1$
	(compiler) (compiler)
25 0.132	1.32 1.18
29 0.162	1.62 1.44
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The dynamic coupled column liquid	(1) commercial product; less than 3% impurities.
chromatography (DCCLC) method was based on generating saturated solu-	-
tions by pumping water through a column packed with glass beads that	(2) distilled over KMnO ₄ and NaOH and passed through a column
have been coated with the component	packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).
(1) (generator column). The con- centration of (1) in the effluent	hass, Filladelphia, Fa).
of the generator column was mea- sured by a modification of the	
coupled column liquid chromato- graphic process that has been	
described in ref 1.	ESTIMATED ERROR:
	temp. ± 0.05°C soly. ± 0.01 mg(1)/kg(2)
[	(standard deviation)
	REFERENCES: 1. May, W.; Chesler, S.; Cram, S.;
	Gump, B.; Hertz, H.; Enagonio, D.;
	Dyszel, S. J. Chromatogr. Sci. 1975, 13, 535.
)	
1	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Rossi, S.S.; Thomas W.H.
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1981</u> , 15, 715-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of pyrene in distilled 0.13 µg/g, corresponding to a mole fra corresponding mass per cent calculated g(1)/100 g sln.	action, $x_1$ , of 6.4 x 10 ⁻¹⁰ . The
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
500 mL of water and an excess of (1) were equilibrated for at least 24 h	<ol> <li>Aldrich; purified by derivati- zation with 2,4,6-trinitrophenol</li> </ol>
in a l L Erlenmeyer flask placed in a constant temperature ( $\pm 0.1^{\circ}C$ ) gyro- tary shaker (200 rpm). After a 12 h stationary equilibration period, 100 mL of saturated solution was drained through a glass-wool plug into a calibrated separatory funnel. Pyrene was isolated from solution by triplicate extraction with 10 mL of hexane (recovery >99%) and determined	(2) Doubly distilled in all-glass apparatus; free of trace organics.
on a Hewlett-Packard Model 5840A gas chromatograph using a WCOTSP-2100	ESTIMATED ERROR:
glass column (30 m x 0.25 mm i.d.). Hydrocarbon concentrations in	Temperature: ±0.1°C Solubility: ±0.01 µg/g (std. dev.
extracts were additionally determined	for 6 determinations)
by UV spectrophotometry (Beckman ACTA MVI). Agreement between GC and UV analyses was typically within 2%. Further details are given in the paper.	REFERENCES:

COMPONENTS: (1) Pyrene; C₁₆H₁₀; [129-00-0] (2) Seawater D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of pyrene (1) in seawater (2) at 298 K has been reported in four works:

Authors	Methods	Salinity g salts/kg sln	10 ⁶ g(1)100 g sln
Krasnoshchekova <i>et al</i> . (ref 1)	spectral	6	7.705
Schwarz (ref 2)	uv spectral	30	9.48
May et al. (ref 3)	HPLC	35	8.60
Rossi and Thomas (ref 4)	GLC	35	8.9

At 298 K and a salinity of 35 g salts/kg sln the data of May *et al*. and Rossi and Thomas are in very good agreement. Since the value reported by May *et al*. is more precise and derived from several measurements using the Setschenow equation, it is adopted as the recommended value for the solubility of pyrene in seawater at the temperature and salinity indicated. Rossi and Thomas and Schwarz each report data over a range of temperatures.

 $\frac{\text{SOLUBILITY OF PYRENE (1) IN SEAWATER (2)}}{\frac{\text{RECOMMENDED VALUE}}{298}}$   $\frac{\text{T/K}}{298}$   $\frac{\text{g salts/kg sln}}{35}$   $\frac{10^6 \text{ g(1)/100 g sln}}{8.60}$ 

#### REFERENCES

- Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. Khim. Tverd. Topl. <u>1977</u>, 11, 133-6.
- 2. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.
- 3. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.
- 4. Rossi, S.S.; Thomas, W.H. Environ. Sci. Technol. 1981, 15, 715-6.

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COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.	
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11, 133-6.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M. Kleinschmidt and D. Shaw	
Salinity: 6 g/kg sln (ref. 1)		
EXPERIMENTAL VALUES:		
The solubility of pyrene in salt water was reported to be 78.9 $\mu$ g/L. The corresponding mass percent and mole fraction, $x_1$ , calculated		
by the compilers are 7.705 x 10 ⁻⁶ g( assuming a solution density of 1.004		
	TUEODU/ETON	
	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1-	Not given.	
L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the		
solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis the solution was taken		
for analysis. The solution was cen- trifuged twice at 7000 g to remove	ESTIMATED ERROR:	
suspended particles. The hydro- carbon was extracted with benzene and	temp. $\pm 1^{\circ}C$ soly. $\pm 2.93$	
concentrated by evaporation, then purified using thin-layer chroma-	type of error not specified	
tography. Spectrometric analysis of an octane solution of the hydro-	REFERENCES :	
carbon was done using the quasili- near luminescence spectra.	<ol> <li>Krasnoshchekova, R.Ya; Guber- grits, M.Ya. Neftekhimiya 1973, 13, 885.</li> </ol>	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Schwarz, F.P.
(2) Sodium chloride; NaCl; [7647-14-5]	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES: Temperature: 8.6-31.1°C	PREPARED BY:
Salinity: 30 g(2)/kg sln	W.Y. Shiu, D. Mackay
EXPERIMENTAL VALUES:	
Solubility of pyrene	in 0.5 g-mol(2)/dm ³
<u>t/°C</u>	<u>10⁷ mol(1)/L sln</u>
8.6	, 2.00
12.2	2.50
15.5	2.85 3.22
18.2 20.7	3.22
23.0	3.90
25.0	4.41
28.1	5.19
31.1	5.96
The corresponding mass percent a calculated by the compilers are 7.97 x 10 ⁻⁹ .	nd mole fraction, $x_1$ , at 25.0°C 9.48 x 10 ⁻⁶ g(1)/100 g sln and
calculated by the compilers are	nd mole fraction, $x_1$ , at 25.0°C 9.48 x 10 ⁻⁶ g(1)/100 g sln and
calculated by the compilers are 7.97 $\times$ 10 ⁻⁹ .	nd mole fraction, $x_1$ , at 25.0°C 9.48 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION
calculated by the compilers are 7.97 $\times$ 10 ⁻⁹ .	9.48 x $10^{-6}$ g(l)/100 g sln and
calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so-	9.48 x 10 ⁻⁶ g(l)/100 g sln and INFORMATION
calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so- lution was determined by fluore- scence and UV absorption measure-	9.48 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS:
calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so- lution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by	9.48 x 10 ⁻⁶ g(l)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %,
calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so- lution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 x 1 cm quartz fluore-	9.48 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ -
calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so- lution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 x 1 cm quartz fluore- scence cell containing 5 mL salt	9.48 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ - NaOH solution and passed
calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so- lution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 x 1 cm quartz fluore- scence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther-	9.48 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ -
calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so- lution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 x 1 cm quartz fluore- scence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its	9.48 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column.
Calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so- lution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 x 1 cm quartz fluore- scence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its fluorescent intensity was measured at 395 nm. The Spectrofluorimeter	9.48 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. ESTIMATED ERROR:
Calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so- lution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 x 1 cm quartz fluore- scence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its fluorescent intensity was measured at 395 nm. The Spectrofluorimeter employed a ratio-photon counting	9.48 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column.
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calculated by the compilers are 7.97 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of pyrene in NaCl so- lution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 x 1 cm quartz fluore- scence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its fluorescent intensity was measured at 395 nm. The Spectrofluorimeter employed a ratio-photon counting mode where pyrene concentration was	<pre>9.48 x 10⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column.</pre>
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	May, W.E.; Wasik, S.P.; Freeman,
(2) Sodium Chloride; NaCl;	D.H.
[7647-14-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of pyrene in aqueous	
reported in terms of the Setschenow	equation:
$\log(S_{O}/S) = K_{S}C_{S}$	
where;	
S _o is the solubility of	of (l) in water (mg/L)
S is the solubility of	f (l) in saline solution (mg/L)
K _s is the Setschenow	constant (L/mol)
C ₂ in the concentration	on of sodium chloride (mol/L)
evaluating the equation for S over the	
$K_{\rm s} = 0.286$ with $S_{\rm o} = 0.132$ .	- 5
s of the second se	
The corresponding mass percent and mole fraction $x_1$ , at salinity =	
35 g(2)/kg sln calculated by the compilers are 8.60 x $10^{-6}$ g(1)/100 g sln	
and 7.84 x $10^{-9}$ .	
AUXILIARY INFORMATION	
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was	(1) greater than 97% pure.
prepared by pumping salt water	
through a "generation column" which was packed with glass beads coated	(2) reagent grade.
with 1% by weight of (1). The saturated solution was extracted	(3) distilled from potassium permanganate-sodium hydroxide
with an "extractor column" packed with a superficially porous bonded	and passed through an XAD-2 column.
C ₁₈ stationary phase, then a water-	column.
ačětonitrile solvent was passed through for extraction. The	
extract was introduced into a liquid chromatograph and the concen-	ESTIMATED ERROR:
tration of (1) was measured with a UV detector.	
	temp ± 0.05°C
	$K_{s} \pm 0.003$
	$K_{s} \pm 0.003$ $S_{0} \pm 0.001$
	$K_{s} \pm 0.003$
	$K_{s} \pm 0.003$ $S_{0} \pm 0.001$
	$K_{s} \pm 0.003$ $S_{0} \pm 0.001$
	$K_{s} \pm 0.003$ $S_{0} \pm 0.001$

NENTS :			

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Rossi, S.S.; Thomas, W.H.
(2) Seawater; natural	Environ. Sci. Technol. <u>1981</u> , 15, 715-6.
VARIABLES:	PREPARED BY:
Temperature: 15 - 25°C	W.Y. Shiu, D. Mackay
Salinity: 35 g/kg sln	•
EXPERIMENTAL VALUES:	
Solubility of py	rene in seawater
	$0^{6}_{Mass%^{a}}$ $10^{9} x_{1}^{a}$ )/100 g sln
15 0.056	5.6 5.1
20 0.071	7.1 6.5
25 0.089	8.9 8.1
^a calculated by compilers	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solution was prepared by equilibrating seawater with an	Pyrene: from Aldrich Chemical Co. and purified with
excess of pyrene for at least 24 hr. in a constant-temperature gyrotary shaker followed by a 12 hr sta-	
tionary equilibration period. A 100 mL aliquot was extracted three	Seawater: collected off Scripps
times with n-hexane. The concen- trated hexane extract was analyzed	Pier and was filtered twice through 0.22 µm membrane and twice ex-
by a gas chromatograph equipped with a flame ionization detector to	tracted with n-hexane then its salinity was adjusted to 35%.
determine the pyrene concentration.	ESTIMATED ERROR:
	Solubility ± 11%
	Temperature ± 0.1°C
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>9,10-Dimethylanthracene;</li> </ol>	Mackay, D.; Shiu, W.Y.
C ₁₆ H ₁₄ ; [781-43-1]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 9,10-dimethylanthra to be 0.056 mg(1) dm ⁻³ sln and $x_1 = 4$	
The corresponding mass percent calcul	ated by the compiler
is 5.6 x $10^{-6}$ g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2)	(1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently	Kodak, or K and K Laboratories, commercial highest grade;
settled at 25°C for at least 48 hrs. Then the saturated solution was	used as received.
decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	
funnel. After shaking for 2 hrs.	
the cyclohexane extract was removed for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given	soly. $\pm$ 0.0005 mg(1) dm ⁻³ sln
in the paper.	(maximum deviation from several determinations).
]	REFERENCES :

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) 2,4,6-Tr: ^C 16 ^H 26;	methyl-2-phenylhept [4810-06-4]	ene; Englin, B.A.; Plate, A.F.; Tugolukov V.M.; Pryanishnikova, M.A.
(2) Water; H	1 ₂ 0; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:		PREPARED BY:
Temperature:	10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALU	JES:	
Solu	bility of Water in	2,4,6-Trimethyl-2-phenylheptene
<u>t</u> ,	/°C g(2)/100	g sln $10^3 x_2$ (compiler)
2	0 0.009 0 0.015 30 0.025	4 1.87
	·····	<u></u>

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:		ORIGINAL MEAS	UREMENTS :	
(1) 7,8-Dimethyltetradeca C ₁₆ H ₃₄ ; [2801-86-7]	ne;		A.; Plate, A.F.; yanishnikova, M.	
(2) Water; H ₂ O; [7732-18-	5]	Khim. Tekh 10, 42-6	nol. Topl. Masel	<u>1965</u> ,
VARIABLES:		PREPARED BY:	<del></del>	
Temperature: 20-50°C		A. Maczyns	ski and M.C. Haul	ait-Pirsor
EXPERIMENTAL VALUES:		L		
Solubility of	water in 7,	8-dimethylt	etradecane	
t/°C	g(2)/10	0 g sln	10 ⁴ x2 (compiler)	
20	0.	0077	9.67	
30	0.	0134	16.83	
40		0219	27.48	
50	0.	0344	43.09	
	AUXILIARY	INFORMATION		
METHOD / AP PARATUS / PROCEDURE :	AUXILIARY		URITY OF MATERIALS:	
Component (1) was introdu	ced into a	SOURCE AND PU		
	ced into a aturated for calcium evolving and hence	SOURCE AND PU	pecified.	
Component (1) was introductive thermostatted flask and so thermostatted flask and so the source with (2). Next, hydride was added and the hydrogen volume measured the concentration of (2)	ced into a aturated for calcium evolving and hence	SOURCE AND PU	pecified.	
thermostatted flask and s 5 hours with (2). Next, hydride was added and the hydrogen volume measured the concentration of (2)	ced into a aturated for calcium evolving and hence	SOURCE AND PU (1) not sp (2) not sp	pecified. pecified. ROR:	
Component (1) was introductive thermostatted flask and so thermostatted flask and so the source with (2). Next, hydride was added and the hydrogen volume measured the concentration of (2)	ced into a aturated for calcium evolving and hence	SOURCE AND PU (1) not sp (2) not sp ESTIMATED ERR	pecified. pecified. ROR:	
Component (1) was introduction thermostatted flask and so thermostatted flask and so the hydride was added and the hydrogen volume measured the concentration of (2)	ced into a aturated for calcium evolving and hence	SOURCE AND PU (1) not sp (2) not sp ESTIMATED ERF not specif	pecified. pecified. ROR:	
Component (1) was introduction thermostatted flask and so thermostatted flask and so the hydride was added and the hydrogen volume measured the concentration of (2)	ced into a aturated for calcium evolving and hence	SOURCE AND PU (1) not sp (2) not sp ESTIMATED ERF not specif	pecified. pecified. ROR:	

COMPONENTS: (1) Hexadecane; C₁₆H₃₄; [544-76-3] (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the hexadecane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1. Quantitative Solubility Studies of the Hexadecane (1) - Water (2) System				
Reference	T/K	Solubility	Method	
Schatzberg (ref 1)	298,313	(2) in (1)	Karl Fischer	
Englin et al. (ref 2)	293-323	(2) in (1)	analytical	
Franks (ref 3)	298	(1) in (2)	GLC	
Yoshida and Yamane (ref 4)	- ^a	(1) in (2)	GLC	
Skripka and Namiot (ref 5)	598 ^b	(2) in (1)	<b>_</b> ^a	
Sutton and Calder (ref 6)	298	(1) in (2)	GLC	
Skripka and Sultanov (ref 7,8)	523-598 ^b	(2) in (1)	_a	

a Not specified.

b Pressure also varied.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. THE SOLUBILITY OF HEXADECANE (1) IN WATER (2)

All data on the solubility of hexadecane in water have probably been obtained at 298 K (Table 1, although Yoshida and Yamane (ref 4) did not specify their temperature). However the values are in poor agreement and no "best" value has been calculated. It may also be noted that all values are higher than the value of  $\sim 2 \times 10^{-9}$  g(1)/100 g sln predicted by extrapolation of lower hydrocarbon solubilities (although whether this extrapolation remains valid for very long chain hydrocarbons is not known).

TABLE	2.	Reported	So	lubi	ility	Values	of
	He	xadecane	(1)	in	Water	(2)	

10 ⁷ g(1)/100 g sln 298 6.3 (ref 3), 5.57 ^b (ref 4), 0.9 (ref 6)	T/K	Reported values ^a
298 6.3 (ref 3), 5.57 ^b (ref 4), 0.9 (ref 6)		10 ⁷ g(1)/100 g sln
298 6.3 (ref 3), 5.57 ^b (ref 4), 0.9 (ref 6)		
	298	6.3 (ref 3), 5.57 ^b (ref 4), 0.9 (ref 6)
	298	6.3 (ref 3), 5.57° (ref 4), 0.9 (ref 6)

b Temperature not specified.

COMPONENTS :	EVALUATOR:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

(continued)

2. THE SOLUBILITY OF WATER (2) IN HEXADECANE (1)

The solubility of water in hexadecane at atmospheric pressure have been reported by Schatzberg (ref 1) and Englin *et al.* (ref 2) over a range of temperatures. However, agreement is poor (Table 3) and the data must be considered as very Tentative.

# TABLE 3. Tentative Solubility Values ofWater (2) in Hexadecane (1)

T/K		Solubi		
	Reported values		"Best" values	(± σ _n ) ^b
	10 ³ g(2)/100 g sl	n	10 ³ g(2)/100 g sln	10 ³ x ₂
293	6.9 (ref 2)		7	0.9
298	5.4 (ref 1), 9.6 a	(ref 2)	8 ± 2	1.0
303	12.3 (ref 2)		12	1.5
313	10.4 (ref 1), 20.9	(ref 2)	$16 \pm 5$	2.0
323	33.2		33	4.2

a Obtained by the Evaluator by graphical interpolation of the authors' data.

b Obtained by averaging where appropriate;  $\sigma_{\rm n}$  has no statistical significance.

At higher pressures the solubility of water in hexadecane has been reported over the range 523-598 K and 1.7-78.5 MPa by Skripka *et al.* (ref 5, 7, 8). As these are the only data available under these conditions no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental values.

## REFERENCES

1.	Schatzberg,	Р.	J.	Phys.	Chem.	<u>1963</u> ,	67,	776-9	•
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- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- 3. Franks, F. Nature (London) 1966, 210, 87-8.
- 4. Yoshida, F.; Yamane, T. Biotechnol. Bioenerg. <u>1971</u>, 13, 691-6.
- 5. Skripka, V.G.; Namiot, A.Yu. Zh. Fiz. Khim. 1974, 48, 782.
- 6. Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u>, 8, 654-7.
- 7. Skripka, V.G.; Tr. Vses. Neftegazov Nauch Issled. Inst. <u>1976</u>, 61, 139-51.
- 8. Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. <u>1973</u>, 47, 1035.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	Schatzberg, P.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.
VARIABLES:	PREPARED BY:
Temperature: 25-40°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
	in heurionna
Solubility of water	
$t/^{\circ}C$ mg(2)/	$\frac{\text{kg sln}}{2}$
25 54	a $6.8 \times 10^{-4}$
40 104	b $13.1 \times 10^{-4}$
a,b See "Estimated Error"	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was saturated by storing over a	(1) Humphrey-Wilkinson, Inc.; ASIM
layer of (2) in a brown glass bottle	normal cetane; passed repeatedly through a column of silica gel
without any agitation. The bottle was sealed with serum cap and com-	until no absorption occurred in
pletely submerged in the water-bath for 7 days. A 20-mL sample was	the 220 to 340 nm spectral range.
withdrawn with a silicone-hydro-	(2) distilled and deionized.
phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted	
to a titer of 1.0-1.3 mg(2)/mL was	
used to titrate (2) in (1) directly in the presence of methanol to a	ESTIMATED ERROR:
"dead-stop" end-point using a Beckman KF3 automatic titrimeter.	temp. ± 0.02°C
Beennan hij adeenaete erermooer	soly. a) 0-6%; b) 0-2% (deviations from the mean)
	REFERENCES:
	REFERENCES:
	[
1	

Components :	ORIGINAL MEASUREMENTS:
<pre>(1) Hexadecane; C₁₆H₃₄; [544-76-3] (2) Water; H₂O; [7732-18-5]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-50°C	A. Maczynski and M.C. Haulait-Pirson

## EXPERIMENTAL VALUES:

## Solubility of water in hexadecane

t/°C	g(2)/100 g sln	$10^{4}x_{2}$ (compiler)
20	0.0069	8.67
30	0.0123	15.45
40	0.0209	26.22
50	0.0332	41.59

AUXILIARY INFORMATION					
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:				
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>				
	ESTIMATED ERROR:				
	not specified.				
	REFERENCES:				

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Herrodocome: $C + \frac{1}{544-76-31}$	Franks, F.
(1) Hexadecane; $C_{16}H_{34}$ ; [544-76-3]	Nature (London) <u>1966</u> , 210, 87-8.
(2) Water; H ₂ O; [7732-18-5]	Nature (Lonaon) <u>1900</u> , 210, 87-8.
VARIABLES :	PREPARED BY:
One temperature: 25°C	F. Kapuku
one temperature. 25 c	r. Napaku
EXPERIMENTAL VALUES:	
The solubility of hexadecane in water	at 25°C was reported to be
in mole fraction $x_1 = 5 \times 10^{-10}$ .	and by the compiler is
The corresponding mass percent calcul $6.3 \times 10^{-7}$ g(1)/100 g sln.	ated by the compiler is
0.7 X 10 g(1//100 g 31	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analysis was performed by gas liquid chromatography. After	<pre>(1) Fluka; purum grade; purity &gt; 97% (chromatographic</pre>
equilibrating the $(1)/(2)$ mixtures	analysis).
in a thermostat, up to 0.5 mL of the aqueous phase was injected into the	(2) not specified.
fractionator fitted to the chroma- tographic column, and (2) was	
removed by "Drierite". The (1)	
concentrations were obtained from the peak areas, after initial	
calibrations.	ESTIMATED ERROR:
	soly. ± 12%
	501y. ± 126
	REFERENCES :

	469
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	Yoshida, F.; Yamane, T.
(2) Water, H ₂ O; [7732-18-5]	Biotechnol. Bioeng. <u>1971</u> , 13, 691-6.
VARIABLES:	PREPARED BY:
One temperature: not specified	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of hexadecane in water $g(1) \text{ cm}^{-3}$ sln.	was reported to be 5.57 x $10^{-9}$
With the assumption that a solution $\dot{c}$ ponding mass percent and mole fraction are 5.57 x $10^{-7}$ g(1)/100 g sln and 4.	on, $x_1$ , calculated by the compiler
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used.	not specified.
10 mL of (1) and 1200 mL of (2) were placed in a stoppered flask and agitated with a magnetic stirrer	
at a speed of 200 rpm for 9 to 24 hrs. (1) was extracted from 1000 ml	
of (2) with 2 mL of heptane and its concentration determined by gas	
chromatography using a Shimadzu equipped with hydrogen flame de-	
tectors.	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS :		ORIGIN	IAL MEASUREMENTS	5:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]		Skripka, V.G.; Namiot, A.Yu.		
(2) Water; H ₂ O; [7732-18-5]		zh.	Fiz. Khim.	<u>1974</u> , <i>48</i> , 782.
VARIABLES :	<u></u>	DDEDAT	NED BY.	
		FREFAI	RED BY:	
One temperature: 325°C Pressure: 1.7-13.18 MPa		A. N	Maczynski	
EXPERIMENTAL VALUES:				
Solubility	of water in	hexad	lecane at 325	°C
p/kg cm ⁻²	p/MPa (compiler)		^x 2	g(2)/100 g sln (compiler)
17.3	1.7		0.083	0.71
41.5	4.07		0.232	2.34
62.5	6.13		0.352	4.14
94.2	9.24		0.517	7.85
134.4	13.18		0.712	16.43
	AUXILIARY	INFORM	ATION	
METHOD/APPARATUS/PROCEDURE:		SOURC	E AND PURITY OF	MATERIALS:
Method was described in r Nothing more was reported paper.		. (1)		specified; CP ed as received.
		(2)	distilled.	
		ESTIM	ATED ERROR:	
		not	specified.	
		1	ENCES:	<u> </u>
		1 1		G.; Skripka, V.G.; Neft. Khoz. <u>1972</u> ,
		2. 8	Sultanov, R.C	.; Skripka, V.G.; Gazov. Delo <u>1972</u> ,
		1	Namiot, A.Yu.	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Hexadecane; C ₁₆ H ₃₄ [544-76-3]	Sutton, C.; Calder, J.A.	
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:	···	
The solubility of hexadecane in wat	or at 25°C was reported to be	
$0.9 \times 10^{-7}$ g(1)/100 g(2) correspond		

 $0.7 \times 10^{-10}$ .

	INFORMATION
METHOD/APPARATUS/PROCEDURE: 175 mg (1) were equilibrated with 700 mL (2) in closed flasks by sha- king on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliguots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane con- taining an internal standard. The	SOURCE AND PURITY OF MATERIALS: (1) Analabs Inc., 99+%. (2) doubly distilled.
concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization de- tectors.	ESTIMATED ERROR: temp. ± 0.1°C soly. ± 16% REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) Hexadecane; C₁₆H₃₄; [544-76-5] (2) Water; H₂0; [7732-18-5]</pre>	Skripka, V.G. Tr. Vses. Neftegazov. Nauch. Issled. Inst. <u>1976</u> , 61, 139-51.		
	Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. <u>1973</u> , 47, 1035.		
VARIABLES:	PREPARED BY:		
Temperature: 250-325°C Pressure: 3.9-78.5 MPa	A. Maczynski		
EXPERIMENTAL VALUES: Solubility of wate	r in hexadecane		
$t/^{\circ}C$ $p/kg cm^{-2}$ $p/MPa$	er)(compiler)		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		
	(continued)		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE: The experimental technique was described in ref 1. No details reported in the paper.	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) source not specified, chemical reagent grade; purity not specified; used as received.</li> <li>(2) distilled.</li> </ul>		
	ESTIMATED ERROR: not specified. REFERENCES: 1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. Gazov. Prom. 1971, 4, 6.		

(1) Hexadecane;  $C_{16}H_{34}$ ; [544-76-5] Skr (2) Water;  $H_2O$ ; [7732-18-5] I

Skripka, V.G.
Tr. Vses. Neftegazov. Nauch. Issled.
Inst. <u>1976</u>, 61, 139-51.
Sultanov, R.G.; Skripka, V.G.
Zh. Fiz. Khim. <u>1973</u>, 47, 1035.

t/°C	<i>P/kg</i> cm ⁻²	<pre>p/MPa (compiler)</pre>	^x 2	g(2)/100 g sln (compiler)
300	93	9.1	0.517	7.84
	100	9.8	0.505	7.51
	134	13.1	0.480	6.84
	1.50	14.7	0.469	6.56
	200	19.6	0.441	5.90
	300	29.4	0.404	5.11
	400	39.2	0.384	4.72
	500	49.0	0.366	4.39
	600	58.8	0.348	4.07
	700	68.6	0.329	3.75
	800	78.5	0.310	3.45
325	134	13.1	0.712	16.43
	150	14.7	0.643	12.53
	200	19.6	0.571	9.57
	300	29.4	0.509	7.62
	400	39.2	0.480	6.84
	500	49.0	0.466	6.49
	600	58.8	0.450	6.11
	700	68.6	0.435	5.77
	800	78.5	0.414	5.32

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COMPONENTS:
 ORIGINAL MEASUREMENTS:
 (1) Hexadecane; C_{16}H_{34}; [544-76-3]
 Sutton, C.; Calder, J.A.
 Environ. Sci. Technol. <u>1974</u>,
8, 654-7.
 (2) Seawater
VARIABLES:
 PREPARED BY:
 One temperature: 25°C
 P.A. Meyers and D. Shaw
 One salinity: 35 g salts/kg sln
EXPERIMENTAL VALUES:
 The solubility of hexadecane in seawater was reported to be
 4 \times 10^{-8} g(1)/100 g sln and x_1 = 3 \times 10^{-11}.
 AUXILIARY INFORMATION
METHOD / APPARATUS / PROCEDURE :
 SOURCE AND PURITY OF MATERIALS:
 (1) and (2) were placed in a glass
 Analabs, Inc., North Haven, Conn.
 stoppered flask fitted with a Teflon
 99 + % pure hydrocarbons.
 stopcock near the bottom. The com-
 Seawater collected from 25 m depth
 ponents were equilibrated by gentle
 in Gulf of Mexico, poisoned with
 shaking for 12 hrs at 25.0 ± 0.1°C
 HgCl<sub>2</sub> sln to prevent bacterial
 The mixture was then allowed to
 growth, and filtered through
 stand for 24 hrs. Samples removed
 Gelman glass fiber filter.
 Na-
 via the stopcock were filtered with
 tural n-alkane levels too low to
 suction through 0.45 \mu m membrane
 cause interference.
 filters to remove any hydrocarbon
 droplets. The filtrate was extrac-
 ted three times with hexane and ana-
 ESTIMATED ERROR: Eight replications were
 lyzed by gas chromatography.
 made. The average of the deviations
of the mean gave an experimental er-
ror of ± 16%, yet some accommodation
may have occurred due to presence of
natural dissolved organic matter.
 REFERENCES:
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[a]fluorene; C ₁₇ H ₁₂ ;	Mackay, D.; Shiu, W.Y.
[238-84-3]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of Benzo[a]fluorene	in water at 25°C was reported
to be 0.045 mg(1) dm ⁻³ sln and $x_1 = 3$	
_	
The corresponding mass percent calcul	lated by the compiler
is 4.5 x $10^{-6}$ g(1)/100 g sln.	
······································	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories,
flask for 24 hrs. and subsequently	commercial highest grade;
settled at 25°C for at least 48 hrs. Then the saturated solution was	used as received.
decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	
funnel. After shaking for 2 hrs.	
the cyclohexane extract was removed for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given	soly. $\pm$ 0.0012 mg(1) dm ⁻³ sln
in the paper.	(maximum deviation from several
	determinations).
	REFERENCES :
1	

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ORIGINAL MEASUREMENTS:
COMPONENTS:
 (1) Benzo[b]fluorene; C17H12;
 Mackay, D.; Shiu, W.Y.
 [243 - 17 - 4]
 J. Chem. Eng. Data 1977, 22,
 399-402.
 (2) Water; H,0; [7732-18-5]
VARIABLES:
 PREPARED BY:
 One temperature: 25°C
 M.C. Haulait-Pirson
EXPERIMENTAL VALUES:
 The solubility of benzo[b]fluorene in water at 25°C was reported
 to be 0.0020 mg(1) dm<sup>-3</sup> sln and x_1 = 9.56 \times 10^{-10}.
 The corresponding mass percent calculated by the compiler
 is 2.0 x 10^{-7} g(1)/100 g sln.
 AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:
 SOURCE AND PURITY OF MATERIALS:
 A saturated solution of (1) in (2) was vigorously stirred in a 250 mL \,
 (1) Aldrich Chemicals, Eastman
 Kodak, or K and K Laboratories,
 flask for 24 hrs. and subsequently
 commercial highest grade;
 settled at 25°C for at least 48 hrs.
 used as received.
 Then the saturated solution was
 decanted and filtered and 50-100 mL
 (2) doubly distilled.
 extracted with approximately 5 mL
 of cyclohexane in a separatory
 funnel. After shaking for 2 hrs.
 the cyclohexane extract was removed
 for analysis. An Aminco-Browman
 spectrophotofluorometer (American
 ESTIMATED ERROR:
 Instruments Ltd.) was used for
 analysis. Many details are given
 soly. \pm 3 \times 10^{-5} mg(1) dm<sup>-3</sup> sln
 in the paper.
 (maximum deviation from several
 determinations).
 REFERENCES :
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COMPONENTS: (1) Benz[a]anthracene; C ₁₈ H ₁₂ ; [56-55-3]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H ₂ O; [7732-18-5]	A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Poland. June 1986.

Quantitative solubility data for benz[a]anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in bena[a]anthracene.

TABLE 1.	Quantitative	Solubility	Studies of
Benz	[a] anthracene	(1) in Wat	er (2)

	<i>т/</i> к	Method
	2, ••	nothou
Davis <i>et al</i> . (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May et al. (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In general the available data are in good agreement given the very low solubility of benz[a]anthracene in water. Although the data of Mackay and Shiu is somewhat higher than all other values there are at the present time insufficient grounds for its rejection. The available data are summarized in Table 2 and may be regarded as Tentative.

TABLE 2.	Tentative :	Solub	<u>ili</u>	ty Val	ues	of
Benz[a	]anthracene	(1)	in N	Water	(2)	

T/K	Solubility values		
	Reported values 10 ⁶ g(1)/100 g sln	"Best" values 10 ⁶ g(1)/100 g sln	
298	0.983 (ref 2), 1.4 (ref 3), 0.94 (ref 4)	1.1 ± 0.2	9
300	1.1 (ref 1)	1.1	9
302	1.22 (ref 4)	1.2	9

a Obtained by averaging where appropriate;  $\sigma_{\rm n}$  has no statistical significance.

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COMPONENTS:
(1) Benz[a]anthracene; C<sub>18</sub>H<sub>12</sub>;
[56-55-3]
(2) Water; H<sub>2</sub>O; [7732-18-5]
(3) EVALUATOR:
EVALUATOR:
G.T. Hefter, School of Mathematical
and Physical Sciences, Murdoch
University, Perth, W.A., Australia.
A. Maczynski, Institute of Physical
Sciences, Warszawa, Poland.
June 1986.
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(continued)

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.
- 4. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Benz[a]anthracene; C₁₈H₁₂; [56-55-3]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108–10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
XPERIMENTAL VALUES:	
Solubility of benz[a]ant	hracene in water
- t/°C	$10^5 g(1) L^{-1} (2)$
27	1.1
	1.1
	1.2
and mole fraction calculated by the $a$ 100 g sln and 8.7 x 10 ⁻¹⁰ .	
100 g sln and 8.7 x 10 ⁻¹⁰ .	
100 g sln and 8.7 x 10 ⁻¹⁰ . AUXILIARY	
100 g sln and 8.7 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in	INFORMATION SOURCE AND PURITY OF MATERIALS;
100 g sln and 8.7 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori-	INFORMATION SOURCE AND PURITY OF MATERIALS; (1) prepared at Harvard University; m.p. range 161.4-161.8°C (cf. ref 2).
100 g sln and 8.7 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 161.4-161.8°C (cf. ref 2). (2) dust-free.
AUXILIARY AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 161.4-161.8°C (cf. ref 2).
100 g sln and 8.7 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 161.4-161.8°C (cf. ref 2). (2) dust-free. ESTIMATED ERROR: town t 2°C
100 g sln and 8.7 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 161.4-161.8°C (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C soly. ± 0.1 x 10 ⁻⁵ g(1) dm ⁻³ (2)

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Benz[a]anthracene; C₁₈H₁₂; [56-55-3] (2) Water; H₂O; [7732-18-5]</pre>	Klevens, H.B. J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson

## EXPERIMENTAL VALUES:

The solubility of benz[a]anthracene in water at 25°C was reported to be  $10^{-5}$  g(1) L⁻¹ sln and 4.31 x  $10^{-8}$  mol(1) L⁻¹ sln. Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 9.83 x  $10^{-7}$  g(1)/ 100 g sln and 7.78 x  $10^{-10}$ .

AUXILIARY INFORMATI	ON
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METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	<ul><li>(1) not specified.</li><li>(2) not specified.</li></ul>
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

	481
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Benz[a]anthracene; C ₁₈ H ₁₂ ;	Mackay, D.; Shiu, W.Y.
[56-55-3]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
	l
EXPERIMENTAL VALUES:	
The solubility of benz[a]anthracene to be 0.014 mg(1) dm ⁻³ sln and $x_1 = 1$	
The corresponding mass percent calcul is 1.4 x $10^{-6}$ g(1)/100 g sln.	ated by the compiler
	······
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories,
flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	commercial highest grade; used as received.
Then the saturated solution was decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. $\pm$ 0.0002 mg(l) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES :

May, W.E.; Wasik, S.P.; Anal. Chem. <u>1978</u> , 50, 9 PREPARED BY: A. Maczynski :[a]anthracene in water 10 ⁶ g(1)/100 g sln (compiler)	97-1000.
A. Maczynski [a]anthracene in water 10 ⁶ g(1)/100 g sln	10
[a]anthracene in water $10^6 g(1)/100 g sln$	
$10^{6}$ g(1)/100 g sln	10
$10^{6}$ g(1)/100 g sln	. 10
10 ⁶ g(1)/100 g sln (commiler)	10
(comprise)	10 ¹⁰ x1 (compiler)
0.94	7.4
1.22	9.6
JARY INFORMATION	
SOURCE AND PURITY OF MATERIALS	; ;
	0.94 1.22 IARY INFORMATION

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

## (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Haas, Philadelphia, Pa).

3% impurities.

ESTIMATED ERROR:

```
temp. ± 0.05°C
soly. \pm 0.001 mg(1)/kg(2) (stand.
 dev.)
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**REFERENCES:** 

1. May, W.; Chesler, S.; Cram, S.; Gump, B; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci. 1975, 13, 535.

COMPONENTS:	EVALUATOR:
<ul> <li>(1) Benz[a]anthracene; C₁₈H₁₂; [55-56-3]</li> <li>(2) Seawater</li> </ul>	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

The solubility of benz[a]anthracene (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10 ⁷ g(l)/100 g sln
Krasnoshchekova <i>et al</i> . (ref 1)	spectral	6	0.62
May et al. (ref 2)	HPLC	35	5.6

The value reported by May *et al*. was derived from several measurements using the Setschenow equation and is consistent with the recommended value for the solubility of benz[a]anthracene in pure water. Therefore their value is adopted as tentative. The value of Krasnoshchekova *et al*. appears slightly low and is considered doubtful.

> SOLUBILITY OF BENZ[A]ANTHRACENE (1) IN SEAWATER (2) TENTATIVE VALUE

T/K	g salts/kg sln	10 ⁷ g(1)/100 g sln
298	35	5.6

## REFERENCES

- Krasnoshchekova, R.Ya.; Pakpill, Yu.A.; Gubergrits, M.Ya. Khim. Tverd. Topl. <u>1977</u>, 11, 133-6.
- May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Benz[a]anthracene; C₁₈H₁₂; [56-55-3]</pre>	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. Khim. Tverd. Topl. 1977, 11(2),
(2) Salt Water	133-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M. Kleinschmidt and D. Shaw
Salinity: 6 g/kg sln (ref. 1)	
EXPERIMENTAL VALUES:	
The solubility of benz[a] anthracene to be 0.63 $\mu$ g/L.	e in salt water was reported
The corresponding mass percent and mo by the compilers are 6.2 x 10 ⁻⁸ g(1)/ assuming a solution density of 1.004	$^{\prime}100 \text{ g sln and } 5.2 \times 10^{-11}$
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was cen- trifuged twice at 7000 g to remove suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma- tography. Spectrometric analysis of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.	ESTIMATED ERROR:

	400		
COMPONENTS :	ORIGINAL MEASUREMENTS:		
<pre>(1) Benz[a]anthracene; C₁₈H₁₂; [56-55-3]</pre>	May, W.E.; Wasik, S.P.; Freeman, D.H.		
(2) Sodium Chloride; NaCl; [7647-14-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.		
(3) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
One temperature: 25°C Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay		
EXPERIMENTAL VALUES:			
The solubility of benz[a]anthracene i			
reported in terms of the Setschenow e	quation:		
log(S _O /S) = K _S C _S			
where;			
S is the solubility of	of (l) in water (mg/L)		
U U	(1) in saline solution (mg/L)		
K _e is the Setschenow c			
5			
5	on of sodium chloride (mol/L)		
evaluating the equation for S over th	e range of $C_{s}$ 0-0.7 mol/L,		
$K_{\rm s} = 0.354$ with $S_{\rm o} = 0.0094$ .			
The corresponding mass percent and mo	the fraction $x_1$ , at salinity =		
35 g(2)/kg sln calculated by the comp	pilers are 5.6 x $10^{-7}$ g(l)/100 g		
$sln$ and 4.5 x $10^{-10}$ .			
AUXILIARY	INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
A saturated solution of (1) was prepared by pumping salt water	(1) greater than 97% pure.		
through a "generation column" which was packed with glass beads coated	(2) reagent grade.		
with 1% by weight of (1). The	(3) distilled from potassium		
saturated solution was extracted with an "extractor column" packed	permanganate-sodium hydroxide and passed through an XAD-2		
with a superficially porous bonded $C_{10}$ stationary phase, then a water-	column.		
acetonitrile solvent was passed			
through for extraction. The extract was introduced into a	)		
liquid chromatograph and the concen- tration of (1) was measured with a	ESTIMATED ERROR:		
UV detector.	temp ± 0.05°C K _s ± 0.002		
	$s_{0} \pm 0.001$		
	REFERENCES:		

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COMPONENTS:	EVALUATOR:
<pre>(1) Chrysene; C₁₈H₁₂; [218-01-9] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry of the Polich Academy of
	Chemistry of the Polish Academy of Sciences, Warszawa, Poland.
	June 1986.

Quantitative solubility data for chrysene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in chrysene.

TABLE 1.	Quantitative Solubil Chrysene (1) in Wate	
Reference	<i>T /</i> K	Method
Davis <i>et al</i> . (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May et al. (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

With the exception of Klevens (ref 2) value at 298K, which is very much higher than other studies (ref 3,4) and is therefore rejected, all the available data are summarized in Table 2 below. The solubilities are in reasonable agreement although their limited number and temperature range suggests a Tentative classification at this stage.

TABLE 2. Tentative Solubility Values forChrysene (1) in Water (2)

Т/К	Solubili	ty values	
	Reported values	"Best" values	
	10 ⁷ g(1)/100 g sln	10 ⁷ g(l)/100 g sln	10 ¹⁰ x1
298	2.0 (ref 3), 1.8 (ref 4)	1.9 ± 0.1	1.5
300	1.5 (ref 1)	1.5	1.2
302	2.2 (ref 4)	2.2	1.7

 $\emph{a}$  Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance.

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(continued next page)

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COMPONENTS:	EVALUATOR:
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch
(2) Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Poland.
	June 1986.
CRITICAL EVALUATION: (continued)	
REFERENCES	
<ol> <li>Davis, W.W.; Krahl, M.E.; Cloves 108-10.</li> </ol>	, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64,
2. Klevens, H.B. J. Phys. Chem. 1	<u>950</u> , <i>54</i> , 283.
3. Mackay, D.; Shiu, W.Y. J. Chem.	Eng. Data <u>1977</u> , 22, 399-402.
4. May, W.E.; Wasik, S.P.; Freeman,	D.H. Anal. Chem. <u>1978</u> , 50, 997-1000.

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COMPONENTS:
 ORIGINAL MEASUREMENTS:
(1) Chrysene; C<sub>18</sub>H<sub>12</sub>; [218-01-9]
 Davis, W.W.; Krahl, M.E.;
 Cloves, G.H.A.
(2) Water; H<sub>2</sub>O; [7732-18-5]
 J. Am. Chem. Soc. 1942, 64,
 108-10.
VARIABLES:
 PREPARED BY:
 M.C. Haulait-Pirson
One temperature: 27°C
EXPERIMENTAL VALUES:
 Solubility of chrysene in water
 10^{6} g(1) L<sup>-1</sup> (2)
 t/°C
 1.5 \pm 0.5
 27
 1.5 \pm 0.2
The best value recommended by the authors is 1.5 \times 10^{-6} q(1) L^{-1} (2).
Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent
and mole fraction, x_1, calculated by the compiler are 1.5 x 10^{-7} g(1)/
100 g sln and 1.2 x 10^{-10}.
 AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:
 SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing
 (1) prepared at Harvard University;
 m.p. range 253.2-253.8°C;
serial dilutions of a suspension
 (cf. ref 2).
of (1) in (2) and determining
nephelometrically the amount of (1) per unit volume beyond which
 (2) dust-free.
further dilution caused no reduc-
tion in light scattering, which
remained equal to that of pure (2).
A Bausch and Lomb Dubosque colori-
meter model 100-mm was employed.
Many details are reported in ref 1.
 ESTIMATED ERROR:
 temp. ± 3°C
 soly. see above
 REFERENCES:

 Davis, W.W.; Parker, Jr., T.V.
J. Am. Chem. Soc <u>1942</u>, 64,

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2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	L
EAPERINE VALUE.	
The solubility of chrysene in water a	t 25°C was reported to be
$6 \times 10^{-6} g(1) L^{-1}$ sln and 2.76 x 10 ⁻⁶ Assuming that 1.00 L sln = 1.00 kg	sln, the corresponding mass percent
and mole fraction, $x_1$ , calculated by	the compiler are 6.29 x $10^{-7}$ g(1)/
100 g sln and 4.98 $\times 10^{-10}$ .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts	(1) not specified.
of (1) in 1 liter of (2) for as long as three months. Aliquots were	(2) not specified.
removed and concentrations deter- mined by spectra.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

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COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	Mackay, D.; Shiu, W.Y.		
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
The solubility of chrysene in water a to be 0.0020 mg(1) dm ⁻³ sln and $x_1 =$ The corresponding mass percent calcul is 2.0 x 10 ⁻⁷ g(1)/100 g sln.	$1.58 \times 10^{-10}$ .		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Brownan spectrophotofluorometer (American Instruments Ltd.) was used for	(2) doubly distilled.		
analysis. Many details are given in the paper.	<pre>soly. ± 0.00017 mg(l) dm⁻³ sln (maximum deviation from several determinations).</pre>		
	REFERENCES :		

	ORIGINAL MEASUREMENTS:		
Components :	ORIGINAL MEASUREMENTS:		
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	May, W.E.; Wasik, S.P.; Freeman, D.		
(2) Water; H ₂ O; [7732-18-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.		
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VARIABLES:	PREPARED BY:		
Temperature: 25 and 29°C	A. Maczynski		
EXPERIMENTAL VALUES:	1		
Solubility of ch	rysene in water		
t/°C mg(1)/kg(2)	$10^7 \text{ g(l)}/100 \text{ g sln}$ $10^{10} x_1$		
	(compiler) (compiler)		
25 0.0018	1.8 1.4		
29 0.0022	2.2 1.7		
	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The dynamic coupled column liquid chromatography (DCCLC) method was	(1) commercial product; less than 3% impurities.		
based on generating saturated solu-			
tions by pumping water through a column packed with glass beads that	(2) distilled over KMnO ₄ and NaOH and passed through a column		
have been coated with the component (1) (generator column). The con-	packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).		
centration of (1) in the effluent	hass, initiaciphia, ia).		
of the generator column was mea- sured by a modification of the			
coupled column liquid chromato- graphic process that has been			
described in ref 1.	ESTIMATED ERROR:		
	temp. ± 0.05°C soly. ± 0.001 mg(1)/kg(2)		
	(standard deviation)		
	REFERENCES:		
	1. May, W.; Chesler, S.; Cram, S.;		
	Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci.		
	<u>1975</u> , <i>13</i> , 535.		

COMPONENTS

COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	May, W.E.; Wasik, S.P.; Freeman,		
(2) Sodium Chloride; NaCl;	D.H.		
[7647-14-5]	Anal. Chem. <u>1978</u> , 50, 997–1000.		
(3) Water; H ₂ O; [7732-18-5]			
VARIABLES: One temperature: 25°C	PREPARED BY:		
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay		
EXPERIMENTAL VALUES: The solubility of chrysene in aqueous	s sodium chloride is		
reported in terms of the Setschenow of			
$\log(S_0/S) = K_SC_S$			
where;			
S is the solubility of	of (l) in water (mg/L)		
j ő	f (l) in saline solution (mg/L)		
K _z is the Setschenow of			
5	on of sodium chloride (mol/L)		
evaluating the equation for S over th			
$K_{s} = 0.336$ with $S_{o} = 0.0018$ .	s 2 2 2 5 5 7 7 2 7 2 7		
s coord with b _o coordinate			
The corresponding mass percent and mo	-		
35 g(2)/kg sln calculated by the comp	pilers are 1.1 x $10^{-7}$ g(1)/100 g sln		
and 8.8 $\times$ 10 ⁻¹¹ .			
AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
A saturated solution of (1) was	(1) greater than 97% pure.		
prepared by pumping salt water through a "generation column" which	(2) reagent grade.		
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium		
saturated solution was extracted	permanganate-sodium hydroxide		
with an "extractor column" packed with a superficially porous bonded	and passed through an XAD-2 column.		
C ₁₈ stationary phase, then a water- acetonitrile solvent was passed			
through for extraction. The extract was introduced into a			
liquid chromatograph and the concen-	ESTIMATED ERROR: temp ± 0.05°C		
tration of (1) was measured with a UV detector.	K _s ± 0.010		
	S ₀ ± 0.0001		
	REFERENCES:		

COMPONENTS: EV	VALUATOR:
<pre>(1) Naphthacene; C₁₈H₁₂; [92-24-0] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

Quantitative solubility data for naphthacene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in naphthacene.

TABLE 1.	Quantitati	ve	Solu	bility	Studies	of
N	aphthacene	(1)	in	Water	(2)	

Reference	T/K	Method
Davis <i>et al</i> .(ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The data are also summarized in Table 2 below. The reported values are in poor agreement. The value of Mackay and Shiu (ref 3) being lower than the other reported values (ref 1,2) is preferred as the Tentative solubility at 298K.

TABLE 2.	Tentativ	e Sol	ubility	Value	of
Naph	thacene (	1) in	Water	(2)	

T/K	Solubility values		
	Reported values 10 ⁸ g(1)/100 g sln	"Best 10 ⁸ g(1)/100 g sln	" value 10 ¹¹ ¤1
298 300	15 ^{<i>a</i>} (ref 2), 5.7 (ref 3) 10 ^{<i>a</i>} (ref 1)	6	5

a Values probably high.

REFERENCES

 Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.

- 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402.

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COMPONENTS :	
	ORIGINAL MEASUREMENTS:
(1) Naphthacene; C ₁₈ H ₁₂ ; [92-24-0]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. 1942, 64,
	108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of naphth	acene in water
	6 g(1) L ⁻¹ (2)
27	$1.0 \pm 0.5$ $1.0 \pm 0.2$
The best value recommended by the aut	hors is $1.0 \times 10^{-6}$ g(1) L ⁻¹ (2).
Assuming that $1.00 \text{ L}$ $sln = 10 \text{ kg}$	
and mole fraction, $x_1$ , calculated by	the compiler are 1.0 x 10 $'$ g(1)/
100 g sln and 7.9 x $10^{-11}$ .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND FURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension	SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 341.5-343.0°C;
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of	<pre>SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University;    m.p. range 341.5-343.0°C;    (cf. ref 2).</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc-	SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 341.5-343.0°C;
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which	<pre>SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University;    m.p. range 341.5-343.0°C;    (cf. ref 2).</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori-	<pre>SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University;    m.p. range 341.5-343.0°C;    (cf. ref 2). (2) dust-free.</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2).	<pre>SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University;    m.p. range 341.5-343.0°C;    (cf. ref 2). (2) dust-free.</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University;   m.p. range 341.5-343.0°C;   (cf. ref 2). (2) dust-free ESTIMATED ERROR:</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University;    m.p. range 341.5-343.0°C;    (cf. ref 2). (2) dust-free. ,</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University;   m.p. range 341.5-343.0°C;   (cf. ref 2). (2) dust-free. , ESTIMATED ERROR: temp. ± 3°C</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 341.5-343.0°C; (cf. ref 2). (2) dust-free. , ESTIMATED ERROR: temp. ± 3°C soly. see above REFERENCES:</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 341.5-343.0°C; (cf. ref 2). (2) dust-free. , (2) dust-free. , ESTIMATED ERROR: temp. ± 3°C soly. see above REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64,</pre>
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University;   m.p. range 341.5-343.0°C;   (cf. ref 2). (2) dust-free. , ESTIMATED ERROR: temp. ± 3°C soly. see above REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V.</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthacene; C ₁₈ H ₁₂ ; [92-24-0]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283–98.
2	
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of naphthacene in wate	r at 25°C was reported to be
$6.6 \times 10^{-9} \text{ mol}(1) \text{ L}^{-1} \text{ sln.}$	
Assuming that $1.00 \text{ L}$ $\sin = 1.00 \text{ kg}$	
and mole fraction calculated by the c sln and 1.2 x $10^{-10}$ .	compiler are 1.5 x 10 ′ g(l)/100 g
sin and 1.2 x 10 .	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts	(1) not specified.
of (1) in 1 liter of (2) for as long as three months. Aliquots were	(2) not specified.
removed and concentrations deter-	
mined by spectra.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Naphthacene; C ₁₈ H ₁₂ ; [92-24-0]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
	M.C. Haulait-Pirson
One temperature: 25°C	M.C. Haulalt-Pirson
EXPERIMENTAL VALUES:	
The solubility of naphthacene in wate to be 0.00057 mg(1) dm ⁻³ sln and $x_1$ The corresponding mass percent calcu is 5.7 x 10 ⁻⁸ g(1)/100 g sln.	$= 3.7 \times 10^{-11}$ .
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.00003 mg(1) dm⁻³ sln (maximum deviation from several determinations).</pre>
	REFERENCES :

COMPONENTS :	EVALUATOR:
<pre>(1) Triphenylene; C₁₈H₁₂; [217-59-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland.
	June 1986.

Quantitative solubility data for triphenylene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in triphenylene.

TABLE 1.	Quantitative	Solut	oility	Studies	of
T	riphenylene (	1) in	Water	(2)	

Reference	T/K	Method
Davis et al. (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The reported data which are summarized in Table 2 are in excellent agreement. However the solubility values are not sufficiently well characterized, at this stage, to justify Recommending the average value.

# TABLE 2. Tentative Solubility Value ofTriphenylene (1) in Water (2)

T/K	Solubili	ty values		
	Reported values	"Best" va	est" value	
	10 ⁶ g(1)/100 g sln	10 ⁶ g(1)/100 g sln	10 ⁹ <i>x</i> 1	
298	4.28 (ref 2), 4.3 (ref 3)	4.3	3.4	
298 300	3.8 ^{<i>a</i>} (ref 1)	-	-	

a Datum not sufficiently well characterized to justify inclusion in "best" values.

#### REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Triphenylene; C ₁₈ H ₁₂ ; [217-59-4]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	L
Solubility of triphe	enylene in water
t/°C 10	5 g(1) $L^{-1}$ (2)
27	3.8 ± 0.8 3.6 ± 0.4
	4.0 ± 0.4
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc-	<ul> <li>(1) prepared at Harvard University; m.p. range 197.5-197.9°C; (cf. ref 2).</li> <li>(2) dust-free.</li> </ul>
tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	
tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori-	ESTIMATED ERROR:
tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	ESTIMATED ERROR: temp. ± 3°C soly. see above

	499
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Triphenylene; C ₁₈ H ₁₂ ; [217-59-4]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
2	
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	l
LAFERINE VALUES.	
The solubility of triphenylene in wa	
4.3 x $10^{-5}$ g(1) L ⁻¹ sln and 1.88 x 1 Assuming that 1.00 L sln = 1.00 kg	
and mole fraction, $x_1$ , calculated by	
100 g sln and 3.39 x $10^{-9}$ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was	(1) not specified.
determined by shaking small amounts of (1) in 1 liter of (2) for as long	(2) not specified.
as three months. Aliquots were removed and concentrations deter-	
mined by spectra.	
	POTIMATED EDDDD
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

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500
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ORIGINAL MEASUREMENTS:
COMPONENTS:
 (1) Triphenylene; C<sub>18</sub>H<sub>12</sub>; [217-59-4]
 Mackay, D.; Shiu, W.Y.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
 J. Chem. Eng. Data 1977, 22,
 399-402.
VARIABLES:
 PREPARED BY:
One temperature: 25°C
 M.C. Haulait-Pirson
EXPERIMENTAL VALUES:
 The solubility of triphenylene in water at 25°C was reported
to be 0.043 mg(1) dm<sup>-3</sup> sln and x_1 = 3.39 \times 10^{-9}.
 The corresponding mass percent calculated by the compiler
 is 4.3 \times 10^{-6} g(l)/100 g sln.
 AUXILIARY INFORMATION
 SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:
A saturated solution of (1) in (2)
 (1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL
 Kodak, or K and K Laboratories,
flask for 24 hrs. and subsequently
 commercial highest grade;
settled at 25°C for at least 48 hrs.
 used as received.
Then the saturated solution was
decanted and filtered and 50-100 mL
 (2) doubly distilled.
extracted with approximately 5 mL
of cyclohexane in a separatory
funnel. After shaking for 2 hrs.
 the cyclohexane extract was removed
for analysis. An Aminco-Browman
spectrophotofluorometer (American
Instruments Ltd.) was used for
 ESTIMATED ERROR:
analysis. Many details are given
 soly. \pm 0.00017 mg(1) dm<sup>-3</sup> sln
in the paper.
 (maximum deviation from several
 determinations).
 REFERENCES:
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COMPONENTS :	EVALUATOR:
(1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

Quantitative solubility data for octadecane (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in octadecane.

TABLE 1.	Quantitative Solubility Studies Octadecane (1) in Water (2)	s of
Reference	T/K	Method
Baker (ref 1)	298-353	radiotracer
Baker (ref 2)	298	radiotracer
Baker (ref 3)	298	not specified
Sutton and Calder (ref	4) 298	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

With the exception of the graphical (ref 1) and v/v data (ref 3) reported by Baker which have been excluded from consideration, all the available data (ref 2,4) are summarized in Table 2 below. The reported values are in poor agreement and both are several orders of magnitude higher than would be predicted by an extrapolation of the lower n-alkane solubilities, viz.  $\sim 10^{-10}$  g(1)/100 g sln, although the validity of this extrapolation is unknown. Nevertheless it must be recognized that the reported values may be substantially in error and no "best" value has been suggested.

## TABLE 2. Reported Values of the Solubility ofOctadecane (1) in Water (2)

<i>T  </i> K	Reported values ⁴ 10 ⁷ g(1)/100 g sln	10 ¹⁰ x ₁
298	6 (ref 2), 2.1 (ref 4) 4.2 (ref 2),	1.5 (ref 4)

a No "best" values suggested because of possible errors in data; see text.

(continued next page)

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COMPONENTS:EVALUATOR:(1) Octadecane; C18H38; [593-45-3]G.T. Hefter, School of Mathematical(2) Water; H20; [7732-18-5]and Physical Sciences, MurdochUniversity, Perth, W.A., Australia.June 1986.
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CRITICAL EVALUATION:

(continued)

REFERENCES

- Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints Symposia 1956, 1, No.2, 5-17.
- Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints <u>1958</u>, 3, No.4, C61-8.
- 3. Baker, E.G. Science 1959, 129, 871-4.
- 4. Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u>, 8, 654-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3]	Baker, E.G.
(2) Water; H ₂ O; [7732-18-5]	Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia <u>1956</u> , 1, N°2, 5-17.
VARIABLES:	PREPARED BY:
Temperature: 5-80°C	M.C. Haulait-Pirson
Temperature. C	
EXPERIMENTAL VALUES:	
The authors reported that the solubil increases from about 55 ppb by weight this amount at 80°C. A graph reporti of the reciprocal absolute temperatur	at room temperature to twice $x_1$ a function
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritio-octadecane was used as radio- active tracer. 0.01 of active (1) was shaken with (2); the mixture was filtered through a 0.05 $\mu$ m fil- ter; 0.01 mL of filtrate was vaporized in hot oxygen and passed over CuO at 600°C; the H ₂ O-T ₂ O derived from the vaporized solvent as well as from the combusted (1) was trapped at -78°C; the melted ice was reduced by Zn and the gas	<ol> <li>(1) tritio-octadecane prepared by hydrogenating octadecene-1 with tritium; 100 curies of tritium were introduced per mole of (1).</li> <li>(2) distilled.</li> </ol>
was counted. Many details are given in the paper.	ESTIMATED ERROR:
J	not specified.
	REFERENCES:

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504
COMPONENTS:
 ORIGINAL MEASUREMENTS:
 (1) Octadecane; C<sub>18</sub>H<sub>38</sub>; [593-45-3]
 Baker, E.G.
 Am. Chem. Soc., Div. Petrol.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
 Chem., Preprints 1958, 3, N°4,
 C61-8.
 VARIABLES:
 PREPARED BY:
 One temperature: 25°C
 M.C. Haulait-Pirson
EXPERIMENTAL VALUES:
 The solubility of octadecane-1,2-H<sup>3</sup> in water at 25°C was reported
 to be 6 x 10^{-9} g(1)/g(2) and that of octadecane-1-C<sup>14</sup> 5.7 x 10^{-9}
 q(1)/q(2).
 The corresponding mass fraction and mole fraction, x_1, calculated by
 the compiler are 6 \times 10^{-7} g(1)/100 g sln and 4 \times 10^{-10}.
 AUXILIARY INFORMATION
 SOURCE AND PURITY OF MATERIALS:
 METHOD/APPARATUS/PROCEDURE:
 (1) Octadecane-1,2-H<sup>3</sup> from Tracer
 Tritiated or carbon-14 labeled (1)
 was used as tracer. The technique
 Lab.; percolated through silica
 of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)-(2) dispersion has been
 qel.
 Octadecane-1-C<sup>14</sup> from Nuclear
 Instrument and Chemical Corpora-
 described in ref 1. A Packard
 tion; used as received.
 Tri-Carb Liquid Scintillation
 Spectrometer was used to detect
 (2) distilled.
 the radioactive (1) dissolved in
 (2).
 ESTIMATED ERROR:
 soly. 20% (standard deviation from
 17 replicate runs).
 REFERENCES:
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1. Baker, E.G. Am. Chem. Soc.,
Div. Petrol. Chem., Preprints-
 Symposia 1956, 1, N°2, 5.
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COMPONENTS :	ORIGINAL MEASUREMENTS:				
(1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3]	Baker, E.G.				
(2) Water; H ₂ O; [7732-18-5]	Science <u>1959</u> , 129, 871-4.				
VARIABLES:	PREPARED BY:				
One temperature: 25°C	F. Kapuku				
	<u></u>				
EXPERIMENTAL VALUES:					
The solubility of octadecane in wate:	r at 25°C was reported to be				
$7.75 \times 10^{-7} \text{ mL}(1)/100 \text{ mL}(2)$ .	-				
AUXILIARY	INFORMATION				
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:				
not specified.	not specified.				
	ESTIMATED ERROR:				
1	not specified.				
	not spectred.				
	REFERENCES :				
1					

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506

506					
COMPONENTS :	ORIGINAL MEASUREMENTS:				
(1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3]	Sutton, C.; Calder, J.A.				
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.				
VARIABLES:	PREPARED BY:				
	M.C. Haulait-Pirson				
One temperature: 25°C	M.C. Radialt-Pirson				
EXPERIMENTAL VALUES:					
The solubility of octadecane in water 2.1 x 10 ⁻⁷ g(1)/100 g(2) correspondin 1.5 x 10 ⁻¹⁰ .					
AUXILIARY	INFORMATION				
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:				
175 mg (1) were equilibrated with 700 mL (2) in closed flasks by sha- king on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane con- taining an internal standard. The concentration of (1) was determined by injection of the hexane extract	<ul> <li>(1) Analabs Inc., 99+%.</li> <li>(2) doubly distilled.</li> </ul> ESTIMATED ERROR:				
into a dual column gas chromatograph equipped with flame ionization de- tectors.					

REFERENCES:

.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3]	Sutton, C.; Calder, J.A.
(2) Seawater	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C One salinity: 35 g salts/kg sln	P.A. Meyers and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of octadecane in seawa 8 x $10^{-8}$ g(1)/100 g sln and $x_1 = 5$ x	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: (1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The com- ponents were equilibrated by gentle shaking for 12 hrs at 25.0 ± 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 µm membrane filters to remove any hydrocarbon droplets. The filtrate was extrac- ted three times with hexane and ana- lyzed by gas chromatography.	<pre>SOURCE AND PURITY OF MATERIALS: Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</pre> ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter. REFERENCES:

HWW 2-HH

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NENTS:
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<pre>Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10. PREPARED BY: M.C. Haulait-Pirson z[a]anthracene in water</pre>
J. Am. Chem. Soc. <u>1942</u> , 64, 108-10. PREPARED BY: M.C. Haulait-Pirson z[a]anthracene in water
M.C. Haulait-Pirson z[a]anthracene in water
M.C. Haulait-Pirson z[a]anthracene in water
z[a]anthracene in water
$\frac{10^5 \text{ g(1) } \text{L}^{-1} \text{ (2)}}{2}$
5.5 ± 0.2
5.4 ± 0.4
5.5 ± 0.2
INFORMATION
SOURCE AND PURITY OF MATERIALS:
<ul> <li>(1) prepared at Harvard University; m.p. range 138.5-139.0°C (cf. ref 2).</li> <li>(2) dust-free.</li> <li>ESTIMATED ERROR: temp. ± 3°C soly. see above</li> <li>REFERENCES:</li> <li>1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101.</li> <li>2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc 1940, 62, 3086.</li> </ul>

	509			
COMPONENTS :	ORIGINAL MEASUREMENTS:			
<pre>(1) 9-Methylbenz[a]anthracene; C₁₉H₁₄; [2381-16-0]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.			
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.			
VARIABLES:	PREPARED BY:			
One temperature: 27°C	M.C. Haulait-Pirson			
EXPERIMENTAL VALUES:	<b>I</b>			
was reported to be 6.6 x $10^{-5}$ g(1) L (Two identical results have been obta With the assumption that 1.00 L slm mass percent and mole fraction, $x_1$ , c 6.6 x $10^{-6}$ g(1)/100 g sln and 4.5 x 1	nined) a = 1.00 kg sln, the corresponding calculated by the compiler are			
	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori-	<ul> <li>(1) prepared at Harvard University; m.p. range 138.0-138.8°C (cf. ref 2).</li> <li>(2) dust-free.</li> </ul>			
meter model 100-mm was employed. Many details are reported in ref 1.				
	ESTIMATED ERROR:			
	temp. $\pm 3^{\circ}$ C soly. $\pm 0.3 \times 10^{-5}$ g(1) dm ⁻³ (2)			
	REFERENCES:			
	<ol> <li>Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. <u>1942</u>, 64, 101.</li> <li>Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1940</u>,</li> </ol>			
	101. 2. Davis, W.W.; Krahl, M.E.; Clove			

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 10-Methylbenz[a]anthracene; C_{19^H14}; [2381-15-9] (2) Water; H₂O; [7732-18-5]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1942, 64,
	108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 10-methylbenz[a]ant was reported to be 5.5 x $10^{-5}$ g(1) L ⁻ (Four identical results have been obt With the assumption that 1.00 L slr mass percent and mole fraction, $x_1$ , c 5.5 x $10^{-6}$ g(1)/100 g sln and 4.1 x l	<pre>1 (2). cained) a = 1.00 kg sln, the corresponding calculated by the compiler are</pre>
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	<ul> <li>(1) prepared at Harvard University; m.p. range 140.0-140.5°C (cf. ref 2).</li> <li>(2) dust-free.</li> </ul>
accurro are reported in rer 1.	ESTIMATED ERROR:
	temp. $\pm 3^{\circ}$ C soly. $\pm 0.5 \times 10^{-5}$ g(l) dm ⁻³ (2)
	REFERENCES:
	<ol> <li>Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. <u>1942</u>, 64, 101.</li> <li>Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1940</u>, 62, 3086.</li> </ol>

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 5-Methylchrysene; C ₁₉ H ₁₄ ;	Davis, W.W.; Krahl, M.E.;		
[3697-24-3]	Cloves, G.H.A.		
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.		
/ARIABLES:	PREPARED BY:		
One temperature: 27°C	M.C. Haulait-Pirson		
XPERIMENTAL VALUES:	I		
Solubility of 5-methylchry	ysene in water		
t/°C 10	$p^{5}$ g(1) $L^{-1}$ (2)		
27	6.5 ± 0.5		
	6.5 ± 0.5		
	5.8 ± 0.5		
	5.5 ± 0.5		
	6.1 ± 0.3		
	6.2 ± 0.3		
With the assumption that 1.00 L sh mass percent and mole fraction, $x_1$ , $\alpha$	n = 1.00 kg sln, the corresponding calculated by the compiler are		
With the assumption that 1.00 L sh mass percent and mole fraction, $x_1$ , $\alpha$	n = 1.00 kg sln, the corresponding calculated by the compiler are		
With the assumption that 1.00 L sh mass percent and mole fraction, $x_1$ , 6 6.2 x 10 ⁻⁶ g(1)/100 g sln and 4.6 x 3	n = 1.00 kg sln, the corresponding calculated by the compiler are		
With the assumption that 1.00 L sh mass percent and mole fraction, $x_1$ , o 6.2 x $10^{-6}$ g(1)/100 g sln and 4.6 x 3 AUXILIARY	n = 1.00 kg sln, the corresponding calculated by the compiler are $10^{-9}$ .		
ÆTHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	n = 1.00 kg sln, the corresponding calculated by the compiler are 10 ⁻⁹ . INFORMATION		
With the assumption that 1.00 L shi mass percent and mole fraction, $x_1$ , o 6.2 x 10 ⁻⁶ g(1)/100 g sln and 4.6 x 3 AUXILIARY ETHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori-	<pre>n = 1.00 kg sln, the corresponding calculated by the compiler are 10⁻⁹. INFORMATION SOURCE AND FURITY OF MATERIALS: (1) prepared at the Ohio State University; m.p. range 117.3-117.7°C; (cf. ref 2).</pre>		

COMPONENTS: (1) Benzo[a]pyrene; C₂₀H₁₂; [50-32-8] (2) Water; H₂O; [7732-18-5] EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for benzo[a]pyrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in benzo[a]pyrene.

TABLE	1. Q	uant	itative	So:	Lubi	llity	Studie	s of
	Benz	o[a]	pyrene	(1)	in	Water	r (2)	

Reference	<i>Т /</i> К	Method
Davis <i>et al</i> . (ref 1)	300	nephelometric
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. It can be seen from Table 2 that the reported solubility values are in good agreement, given that they have been measured at slightly different temperatures. However, further studies are required before any data can be Recommended.

TABLE 2.	Tentative	Solubility	Values of
Benzo	o[a]pyrene	(1) in Wat	er (2)

T/K		Solubility values	
	Reported values	"Best" va	
	10 ⁷ g(1)/100 g sln	10 ⁷ g(1)/100 sln	10 ¹⁰ x ₁
298	3.8 (ref 2)	3.8	2.7
300	4.0 (ref 1)	4.0	2.9

REFERENCES

 Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.

2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Benzo[a]pyrene; C ₂₀ H ₁₂ ; [50-32-8]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108–10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	L
Solubility of benzo	p[a]pyrene in water
t/°C	$10^{6} g(1) L^{-1} (2)$
27	$3.0 \pm 0.5$ $4.5 \pm 0.5$ $4.0 \pm 0.1$ $4.0 \pm 0.5$ $3.5 \pm 0.5$
The best value recommended by the aut With the assumption that 1.00 L shr mass percent and mole fraction calcul $4.0 \times 10^{-7}$ g(1)/100 g sln and 2.9 x 1	h = 1.00 kg sln, the corresponding Lated by the compiler are
With the assumption that 1.00 L slm mass percent and mole fraction calcul	h = 1.00 kg sln, the corresponding Lated by the compiler are
With the assumption that 1.00 L sh mass percent and mole fraction calcul $4.0 \times 10^{-7} \text{ g(1)}/100 \text{ g sln and 2.9 x }$	h = 1.00 kg sln, the corresponding Lated by the compiler are $10^{-10}$ .
With the assumption that 1.00 L sh mass percent and mole fraction calcul $4.0 \times 10^{-7} \text{ g(1)/100 g shn and 2.9 x 1}$	h = 1.00 kg sln, the corresponding Lated by the compiler are
With the assumption that 1.00 L slm mass percent and mole fraction calcul 4.0 x 10 ⁻⁷ g(1)/100 g sln and 2.9 x 1 AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>h = 1.00 kg sln, the corresponding lated by the compiler are 10⁻¹⁰. INFORMATION SOURCE AND FURITY OF MATERIALS: (1) Hoffman La-Roche; used as received; m.p. range 176.3-177.0°C, (cf. ref 2). (2) dust-free.</pre>
With the assumption that 1.00 L slm mass percent and mole fraction calcul 4.0 x 10 ⁻⁷ g(1)/100 g sln and 2.9 x 1 AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori-	<pre>h = 1.00 kg sln, the corresponding lated by the compiler are 10⁻¹⁰. INFORMATION SOURCE AND FURITY OF MATERIALS: (1) Hoffman La-Roche; used as received; m.p. range 176.3-177.0°C, (cf. ref 2). (2) dust-free. ESTIMATED ERROR:</pre>
With the assumption that 1.00 L slm mass percent and mole fraction calcul 4.0 x 10 ⁻⁷ g(1)/100 g sln and 2.9 x 1 AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>h = 1.00 kg sln, the corresponding lated by the compiler are 10⁻¹⁰. INFORMATION SOURCE AND FURITY OF MATERIALS: (1) Hoffman La-Roche; used as received; m.p. range 176.3-177.0°C, (cf. ref 2). (2) dust-free.</pre>
With the assumption that 1.00 L slm mass percent and mole fraction calcul 4.0 x 10 ⁻⁷ g(1)/100 g sln and 2.9 x 1 AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	<pre>h = 1.00 kg sln, the corresponding lated by the compiler are 10⁻¹⁰. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Hoffman La-Roche; used as received; m.p. range 176.3-177.0°C, (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C</pre>

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COMPONENTS:
 ORIGINAL MEASUREMENTS:
 (1) Benzo[a]pyrene; C<sub>20</sub>H<sub>12</sub>;
 Mackay, D.; Shiu, W.Y.
 [50 - 32 - 8]
 J. Chem. Eng. Data 1977, 22,
 399-402.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
VARIABLES:
 PREPARED BY:
 M.C. Haulait-Pirson
 One temperature: 25°C
EXPERIMENTAL VALUES:
 The solubility of benzo[a]pyrene in water at 25°C was reported
 to be 0.0038 mg(1) dm<sup>-3</sup> sln and x_1 = 2.73 \times 10^{-10}.
 The corresponding mass percent calculated by the compiler
 is 3.8 \times 10^{-7} q(1)/100 q sln.
 AUXILIARY INFORMATION
METHOD / APPARATUS / PROCEDURE :
 SOURCE AND PURITY OF MATERIALS:
 A saturated solution of (1) in (2)
 (1) Aldrich Chemicals, Eastman
 was vigorously stirred in a 250 mL
 Kodak, or K and K Laboratories,
 flask for 24 hrs. and subsequently
 commercial highest grade;
 settled at 25°C for at least 48 hrs.
 used as received.
 Then the saturated solution was
 decanted and filtered and 50-100 mL
 (2) doubly distilled.
 extracted with approximately 5 mL
 of cyclohexane in a separatory
 funnel. After shaking for 2 hrs.
 the cyclohexane extract was removed
 for analysis. An Aminco-Browman
 spectrophotofluorometer (American
 Instruments Ltd.) was used for
 ESTIMATED ERROR:
 analysis. Many details are given
 soly. \pm 0.00031 mg(1) dm<sup>-3</sup> sln
 in the paper.
 (maximum deviation from several
 determinations).
 REFERENCES :
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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Benzo[a]pyrene; C₂₀H₁₂; [50-32-8]</pre>	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. Khim. Tverd. Topl. 1977, 11,
(2) Salt Water	133-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M. Kleinschmidt and D. Shaw
Salinity: 6 g/kg sln (ref. 1)	
EXPERIMENTAL VALUES:	
The solubility of benzo[a]pyrene in to be 0.13 $\mu$ g/L. The corresponding mass percent and m	ole fraction, $x_1$ , calculated
by the compilers are 1.3 x $10^{-8}$ g(1) assuming a solution density of 1.004	
assuming a solution density of 1.004	лg/ ц.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken	
for analysis. The solution was cen- trifuged twice at 7000 g to remove	ESTIMATED ERROR:
suspended particles. The hydro-	+ amp + 180
carbon was extracted with benzene and concentrated by evaporation, then	soly. ± 0.008
purified using thin-layer chroma- tography. Spectrometric analysis	type of error not specified
tography. Spectrometric analysis of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.	REFERENCES: 1. Krasnoshchekova, R.Ya; Guber- grits, M.Ya. Neftekhimiya <u>1973</u> ,
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[e]pyrene; C ₂₀ H ₁₂ ; [192-97-2]	Schwarz, F.P.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
VARIABLES:	PREPARED BY:
Temperature: 8.6-31.7°C	A. Maczynski
EXPERIMENTAL VALUES:	·····
Solubility of benzo[6	e]pyrene in water
t/°C 10 ⁸ mol(1) L	$10^7$ g(l)/100 g sln $10^{10}x_1$ (compiler) (compiler)
$\frac{1.29 \pm 0.07}{1.29 \pm 0.07}$	3.25 2.32
$14.0$ $1.42 \pm 0.05$	3.58 2.56
$17.0$ $1.76 \pm 0.13$	4.44 3.17
17.5 $1.56 \pm 0.08$	3.94 2.81
20.0 1.82 ± 0.09	4.59 3.28
20.2 1.90 ± 0.14	4.79 3.42
23.0 2.01 ± 0.20	5.07 3.62
23.2 2.12 ± 0.10	5.35 3.82
29.2 2.55 ± 0.02	6.43 4.59
31.7 2.70 ± 0.15	6.81 4.86
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Two methods were used. At 25°C the solubility of (1) in (2)	(1) source not specified; better than 99 mole%, by glc; used as received.
was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectro- fluorimetry method was used.	(2) distilled over KMnO ₄ and NaOH and passed through a Sephadex column.
The sealed fluorescence cells con- tained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then	ESTIMATED ERROR:
removed, quickly wiped dry and placed in the fluorimeter.	temp. ± 0.1°C soly. see above
	REFERENCES:

COMPONENTS:		EVALUATOR:	
(1) Benzo[e]pyrene; C ₂₀ H [192-97-2]	12'	D.G. Shaw Institute of Mar University of Al	
(2) Seawater		Fairbanks, Alask	
		December 1982	
CRITICAL EVALUATION:	· · · · · · · · · · · · · · · · · ·		
reported in two works: Authors	Method	Salinity g salts/kg sln	10 ⁷ g(1)/100 g sln
Krasnoshchekova <i>et al.</i> (ref 1)	spectral	6	1.79
	uv spectral		2 22
Schwarz (ref 2)	uv spectrur	30	3.32
	-		
Schwarz (ref 2) The two reported values adopted as tentative at	are in fair a	greement and there	fore both are
The two reported values	are in fair a their respect	greement and there ive salinities. S	fore both are

	TENTATIVE VALUES	
T/K	g salts/kg sln	10 ⁷ g(1)/100 g sln
298	б	1.79
298	30	3.32

### REFERENCES

1. Krasnoshchekova, R.Ya.; Pakpill, Yu.A; Gubergrits, M.Ya. Khim. Tverd. Topl. <u>1977</u>, 11, 133-6.

2. Schwarz, F.P. J. Chem. Eng. Data <u>1977</u>, 22, 273-7.

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Benzo[e]pyrene; C₂₀H₁₂; [192-97-2]</pre>	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11, 133-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M. Kleinschmidt and D. Shaw
Salinity: 6 g/kg sln (ref. 1)	
EXPERIMENTAL VALUES:	· · · · · · · · · · · · · · · · · · ·
The solubility of Benzo[e]pyrene in to be 1.83 µg/L. The corresponding mass percent and m by the compilers are 1.79 x 10 ⁻⁷ g(1 assuming a solution density of 1.004	tole fraction, $x_1$ , calculated )/100 g sln and 1.34 x 10 ⁻¹⁰
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was cen- trifuged twice at 7000 g to remove suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma- tography. Spectrometric analysis of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.	ESTIMATED ERROR:

COMPONENTS:	ORIGINAL MEASUREMENTS:
	Schwarz, F.P.
(1) Benzo[e]pyrene; C ₂₀ H ₁₂ ; [192-97-2]	
<pre>(2) Sodium chloride; NaCl; [7647-14-5]</pre>	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 8.9-30.2°C	W.Y. Shiu, D. Mackay
Salinity: 30 g(2)/kg sln	
EXPERIMENTAL VALUES:	
Solubility of benzo[e]py	rene in 0.5 mol(2)/L
<u>t/°C</u>	10 ⁸ mol(1)/L sln
8.9	0.82
10.8	0.88
15.6	1.01
17.0	1.01
19.2	1.04
21.7	1.13
25.3	1.35
27.1	1.42
30.2	1.66
$2.44 \times 10^{-10}$ .	
AUXILIARY	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
The solubility of benzo[e]pyrene in	
	SOURCE AND PURITY OF MATERIALS:
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence	SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade,
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of	SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1	SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 -
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column,</pre>
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade.</pre>
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec-	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR:</pre>
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea-	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author)</pre>
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author) Temperature ± 0.1°C (author)</pre>
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author)</pre>
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of benzo[e]pyrene in	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author) Temperature ± 0.1°C (author)</pre>
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of benzo[e]pyrene in cyclohexane therefore provide an absolute solubility scale for the	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author) Temperature ± 0.1°C (author)</pre>
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of benzo[e]pyrene in cyclohexane therefore provide an	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author) Temperature ± 0.1°C (author)</pre>
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of benzo[e]pyrene in cyclohexane therefore provide an absolute solubility scale for the	<pre>SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity &gt; 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author) Temperature ± 0.1°C (author)</pre>

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Cholanthrene; C ₂₀ H ₁₄ ; [479-23-2]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of cholanthrene in wat $3.5 \times 10^{-6} g(1) L^{-1}$ (2). (Two identi- With the assumption that 1.00 L slm mass percent and mole fraction, $x_1$ , c $3.5 \times 10^{-7} g(1)/100 g sln and 2.5 \times 10^{-7}$	cal results were obtained). a = 1.00 kg sln, the corresponding calculated by the compiler are
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	<ul> <li>(1) prepared at Harvard University; m.p. range 170.1-170.6°C; (cf. ref 2).</li> <li>(2) dust-free.</li> </ul>
Many details are reported in fer 1.	ESTIMATED ERROR:
	temp. $\pm 3^{\circ}$ C soly. $\pm 0.5 \times 10^{-6}$ g(1) dm ⁻³ (2)
	REFERENCES:
	<ol> <li>Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. <u>1942</u>, 64, 101.</li> <li>Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc.</li> </ol>
	<u>1940</u> , <i>62</i> , 3086.

<pre>flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.</pre> commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. (2) doubly distilled. (2) doubly distilled. (3) doubly distilled. (4) doubly distilled. (5) doubly distilled. (2) doubly distilled. (3) doubly distilled. (4) doubly distilled. (5) doubly distilled. (6) doubly distilled. (6) doubly distilled. (7) doubly distilled. (8) doubly distilled. (9) doubly	COMPONENTS :	ORIGINAL MEASUREMENTS:
(2) Water: $H_2O; [7732-18-5]$ 399-402.         VARIABLES:       PREPARED BY:         One temperature: 25°C       M.C. Haulait-Pirson         EXPERIMENTAL VALUES:       M.C. Haulait-Pirson         The solubility of 7,12-dimethylbens[a]anthracene in water at 25°C         was reported to be 0.061 mg(1) dm ⁻³ sln and $x_1 = 4.26 \times 10^{-9}$ .         The corresponding mass percent calculated by the compiler         is 6.1 x 10 ⁻⁶ g(1)/100 g sln.         METHOD/APPARATUS/PROCEDURE:         A saturated solution of (1) in (2)         was vigorously stirred in a 250 mL         flask for 24 hrs. and subsequently         settled at 25°C for at least 48 hrs.         Then the saturated solution was         decanted and filtered and 50-100 mL         extracted with approximately 5 mL         florelokane in a separatory         funel. After shaking for 2 hrs.         the cyclohexane extract was removed         spectrophotoflucometer (American Instruments Ltd.) was used for         malysis. Many details are given         in the paper.	<ol> <li>7,12-Dimethylbenz[a]anthracene;</li> </ol>	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ 0; [7732-18-5]         VARIABLES:         One temperature: 25°C         The solubility of 7,12-dimethylbenz[a]anthracene in water at 25°C         was reported to be 0.061 mg(1) dm ⁻³ sin and x ₁ = 4.26 x 10 ⁻⁹ .         The corresponding mass percent calculated by the compiler         is 6.1 x 10 ⁻⁶ g(1)/100 g sln.         Source AND FURITY OF MATERIALS:         A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently setted and 25°r or a Least 48 hrs. Then the saturated solution was the or of 0.10 mL of cyclebrase in a seperatory finnel. After a mather of 15° mL or or shaking for 2.100 mL deviation stir.) was removed for analysis. Mand mather of thoman spectrophote luorometer (American Instuments 5td.) was subsequent (American Instuments 5td.) was removed for analysis. Many details are given in the paper.       Source AND FURITY OF MATERIALS:         (1) Aldrich Chemicals, Eastman was vigorously stirred in a 250 mL or ophotex and in a subsequently sused as received.         Source AND FURITY OF MATERIALS:         (2) doubly distilled.         Source AND FURITY OF MATERIALS:         Source AND FURITY OF MATERIALS:         (1) Aldrich Chemicals, Eastman was removed for analysis. Many details are given in the paper.	C ₂₀ H ₁₆ ; [57-97-6]	
One temperature: $25^{\circ}$ C       M.C. Haulait-Pirson         EXPERIMENTAL VALUES:       M.C. Haulait-Pirson         The solubility of 7,12-dimethylbenz[a]anthracene in water at $25^{\circ}$ C was reported to be 0.061 mg(1) dm ⁻³ sln and $x_1 = 4.26 \times 10^{-9}$ .         The corresponding mass percent calculated by the compiler is 6.1 x $10^{-6}$ g(1)/100 g sln.         METHOD/APPARATUS/FROCEDURE:         A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25° C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (Marcican Instruments Ltd.) was used for analysis. Many details are given in the paper.       Source AND PURITY OF MATERIALS:         ESTIMATED ERROR:       (aubly distilled.	(2) Water; H ₂ O; [7732-18-5]	399-402.
One temperature: 25°C       M.C. Haulait-Pirson         EXPERIMENTAL VALUES:         The solubility of 7,12-dimethylbenz[a]anthracene in water at 25°C         was reported to be 0.061 mg(1) dm ⁻³ sln and $x_1 = 4.26 \times 10^{-9}$ .         The corresponding mass percent calculated by the compiler         is 6.1 x 10 ⁻⁶ g(1)/100 g sln.         METHOD/APPARATUS/FROCEDURE:         A saturated solution of (1) in (2)         was vigorously stirred in a 250 mL         flask for 24 hrs. and subsequently         settacted and filtered and 50-100 mL         extracted with approximately 5 mL         of cyclohexane extract was removed         for analysis. An Aminco-Browman         spectrophotofluorometer (American         Instruments Ltd.) was used for         analysis. Many details are given         in the paper.	-	
EXPERIMENTAL VALUES:         The solubility of 7,12-dimethylbenz[a]anthracene in water at 25°C was reported to be 0.061 mg(1) dm ⁻³ sln and $x_1 = 4.26 \times 10^{-9}$ .         The corresponding mass percent calculated by the compiler is 6.1 x $10^{-6}$ g(1)/100 g sln.         AUXILIARY INFORMATION         METHOD/APPARATUS/PROCEDURE:         A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. Many details are given in the paper.       Source and pull distilled.         ESTIMATED ERROR:       Soly. ± 0.0006 mg(1) dm ⁻³ sln (maximu deviation from several	VARIABLES:	PREPARED BY:
The solubility of 7,12-dimethylbenz[a]anthracene in water at 25°C was reported to be 0.061 mg(1) dm ⁻³ sln and $x_1 = 4.26 \times 10^{-9}$ . The corresponding mass percent calculated by the compiler is 6.1 x 10 ⁻⁶ g(1)/100 g sln. <b>AUXILIARY INFORMATION</b> <b>METHOD/APPARATUS/PROCEDURE:</b> A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. Many details are given in the paper. <b>SUMCE AND FUNITY OF MATERIALS:</b> <b>SURCE AND FUNITY OF MATERIALS:</b> (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories commercial highest grade; used as received. (2) doubly distilled. <b>ESTIMATED ERROR:</b> (3) $t = 0.0006 mg(1) dm-3 sln (maximum deviation from several)$	One temperature: 25°C	M.C. Haulait-Pirson
Was reported to be 0.061 mg(1) dm ⁻³ sln and $x_1 = 4.26 \times 10^{-9}$ .         The corresponding mass percent calculated by the compiler is 6.1 x 10 ⁻⁶ g(1)/100 g sln.         AUXILIARY INFORMATION         METHOD/APPARATUS/PROCEDURE:         A saturated solution of (1) in (2) was vigorously stirred in a 250° List the saturated solution was idecanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. Maninco-Browman spectrophotoflucormeter (American Instruments Ltd.) was used for analysis. Many details are given in the paper.       Source AND FURITY OF MATERIALS:         (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories commercial highest grade; used as received.         (2) doubly distilled.	EXPERIMENTAL VALUES:	
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.SOURCE AND PURITY OF MATERIALS:Source and purchase (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories commercial highest grade; used as received.(2) doubly distilled.(2) doubly distilled.(2) doubly distilled.(2) doubly distilled.(3) After shaking for 2 hrs. the cyclohexane extract was removed for analysis. Many details are given in the paper.(4) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories commercial highest grade; used as received.(2) doubly distilled.(2) doubly distilled.(2) doubly distilled.(3) ESTIMATED ERROR: (maximum deviation from several	was reported to be 0.061 mg(1) dm ⁻³ s The corresponding mass percent calcul	ln and $x_1 = 4.26 \times 10^{-9}$ .
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. 		
<ul> <li>A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.</li> <li>(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories commercial highest grade; used as received.</li> <li>(2) doubly distilled.</li> <li>(2) doubly distilled.</li> </ul>		INFORMATION
REFERENCES:	A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given	<ul> <li>(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.</li> <li>(2) doubly distilled.</li> <li>ESTIMATED ERROR: soly. ± 0.0006 mg(1) dm⁻³ sln (maximum deviation from several determinations).</li> </ul>

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 9,10-Dimethylbenz[a]anthracene; C₂₀H₁₆; [56-56-4]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of 9,10-dimethylbe	nz[a]anthracene in water
<i>t</i> /°C	$10^5$ g(1) L ⁻¹ (2)
27	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$
mass percent and mole fraction, $x_1$ , c	alculated by the compiler are
-	alculated by the compiler are
mass percent and mole fraction, $x_1$ , c 4.3 x 10 ⁻⁶ g(1)/100 g sln and 3.0 x 1	alculated by the compiler are
mass percent and mole fraction, $x_1$ , c 4.3 x 10 ⁻⁶ g(1)/100 g sln and 3.0 x 1 AUXILIARY	alculated by the compiler are 0 ⁻⁹ .
AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	alculated by the compiler are 0 ⁻⁹ . INFORMATION
mass percent and mole fraction, $x_1$ , or $4.3 \ge 10^{-6}$ g(1)/100 g sln and 3.0 $\ge 1$ AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori-	alculated by the compiler are 0 ⁻⁹ . INFORMATION SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 122.6-122.9°C (cf. ref 2). (2) dust-free. ESTIMATED ERROR:
mass percent and mole fraction, $x_1$ , or $4.3 \ge 10^{-6}$ g(1)/100 g sln and 3.0 $\ge 1$ AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	alculated by the compiler are 0 ⁻⁹ . INFORMATION SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 122.6-122.9°C (cf. ref 2). (2) dust-free.

COMPONENTS :	
	ORIGINAL MEASUREMENTS:
<pre>(1) 10-Ethylbenz[a]anthracene; C₂₀H₁₆; [14854-08-1]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	I
Solubility of 10-ethylber	nz[a]anthracene in water
t/°C	$10^5$ g(1) L ⁻¹ (2)
The best value recommended by the au With the assumption that 1.00 L slimass percent and mole fraction, $x_1$ , 4.5 x 10 ⁻⁶ g(1)/100 g sln and 3.2 x	n = 1.00 kg sln, the corresponding calculated by the compiler are
AUXILIARY	INFORMATION
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per	<pre>(1) prepared at Harvard University; m.p. range 112.4-112.8°C (cf. ref 2).</pre>

	525
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Eicosane; C ₂₀ H ₄₂ ; [112-95-8]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of eicosane in water a 1.9 x 10 ⁻⁷ g(1)/100 g(2) correspondin 1.1 x 10 ⁻¹⁰ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
175 mg (1) were equilibrated with 700 mL (2) in closed flasks by sha- king on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane con- taining an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization de- tectors.	<ul> <li>(1) Analabs Inc., 99+%.</li> <li>(2) doubly distilled.</li> </ul> ESTIMATED ERROR:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Eicosane; C ₂₀ H ₄₂ ; [112-95-8]	Sutton, C.; Calder, J.A.
(2) Seawater	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C One salinity: 35 g salts/kg sln	P.A. Meyers and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of eicosane in seawate 8 x $10^{-8}$ g(1)/100 g sln and $x_1 = 5$ x	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The com- ponents were equilibrated by gentle shaking for 12 hrs at 25.0 $\pm$ 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 $\mu$ m membrane filters to remove any hydrocarbon droplets. The filtrate was extrac- ted three times with hexane and ana- lyzed by gas chromatography.	<pre>Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</pre> ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter. REFERENCES:

OMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 5-Methylbenzo[a]pyrene; C_{21H14}; [2319-96-2]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
/ARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	I
Solubility of 5-methylber	zo[a]pyrene in water
 t/°C	$10^7 g(1) L^{-1} (2)$
27	8 ± 2
	10 ± 4
	8 ± 2
8 x $10^{-8}$ g(1)/100 g sln and 6 x $10^{-11}$	•
8 x 10 ⁻⁸ g(1)/100 g sln and 6 x 10 ⁻¹¹	•
	INFORMATION
8 x 10 ⁻⁸ g(1)/100 g sln and 6 x 10 ⁻¹³ AUXILIARY METHOD/APPARATUS/PROCEDURE:	
AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori-	INFORMATION SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 216.6-217.3°C (cf. ref 2). (2) dust-free. ESTIMATED ERROR:
AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	INFORMATION SOURCE AND FURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 216.6-217.3°C (cf. ref 2). (2) dust-free.

COMPONENTS: (1) 3-Methylcholanthrene; C₂₁H₁₆; [56-49-5] (2) Water; H₂O; [7732-18-5] EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for 3-methylcholanthrene (1) in water (2) have been reported in the publications listed in Table 1. No data are available on the solubility of water in 3-methylcholanthrene.

## TABLE 1. Quantitative Solubility Studies of3-Methylcholanthrene (1) in Water (2)

Reference	T/K	Method
Davis et al. (ref 1)	300	nephelometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. Unfortunately, the available data, obtained at slightly different temperatures are in poor agreement. Although the values of Mackay and Shiu (ref 2) are generlly more reliable than those of Davis *et al.* (ref 1) the system is not sufficiently well-characterized to justify a preference at this stage and no "best" values have been nominated.

TABLE 2.	Reported	Solub	ility	Value	s of
3-Methyl	cholanthre	ene (1	) in	Water	(2)

T/K	Reported va	lues ^a
	10 ⁷ g(1)/100 g sln	10 ¹⁰ x ₁
298	2.9 (ref 2)	1.9 (ref 2)
300	1.5 (ref 1)	1.0 (ref 1)

a No "best" values nominated because of uncertainties in the available data, see text.

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402.

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 3-Methylcholanthrene; C_{21^H16}; [56-49-5]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108–10.
VARIABLES:	PREPARED BY:
One temperature: 27°C M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:	
Solubility of 3-methylch	nolanthrene in water
t/°C 10	$p^{6}$ g(1) $L^{-1}$ (2)
27	1.3
	1.8
	1.8
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining	<pre>(1) Hoffman La-Roche; used as received;</pre>
nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	<pre>m.p. range 175.3-177.1°C; (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C soly. ± 0.3 x 10⁻⁶ g(1) dm⁻³(2)</pre>

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ORIGINAL MEASUREMENTS:
COMPONENTS:

 3-Methylcholanthrene; C<sub>21</sub>H<sub>16</sub>;

 Mackay, D.; Shiu, W.Y.
 [56 - 49 - 5]
 J. Chem. Eng. Data 1977, 22,
 399-402.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
VARIABLES:
 PREPARED BY:
 One temperature: 25°C
 M.C. Haulait-Pirson
EXPERIMENTAL VALUES:
 The solubility of 3-methylcholanthrene in water at 25°C was reported
 to be 0.0029 mg(1) dm<sup>-3</sup> sln and x_1 = 1.92 \times 10^{-10}.
 The corresponding mass percent calculated by the compiler
 is 2.9 \times 10^{-7} \text{ g(l)}/100 \text{ g sln.}
 AUXILIARY INFORMATION
 METHOD/APPARATUS/PROCEDURE:
 SOURCE AND PURITY OF MATERIALS:
 A saturated solution of (1) in (2)
 (1) Aldrich Chemicals, Eastman
 was vigorously stirred in a 250 mL
 Kodak, or K and K Laboratories,
 flask for 24 hrs. and subsequently
 commercial highest grade;
 settled at 25°C for at least 48 hrs.
 used as received.
 Then the saturated solution was
 decanted and filtered and 50-100 mL
 (2) doubly distilled.
 extracted with approximately 5 mL
 of cyclohexane in a separatory
 funnel. After shaking for 2 hrs.
 the cyclohexane extract was removed
 for analysis. An Aminco-Browman
 spectrophotofluorometer (American
 Instruments Ltd.) was used for
 ESTIMATED ERROR:
 analysis. Many details are given
 soly. \pm 0.000021 mg(1) dm<sup>-3</sup> sln
 in the paper.
 (maximum deviation from several
 determinations).
 REFERENCES:
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COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Benzo[ghi]perylene; C₂₂H₁₂;</pre>	Mackay, D.; Shiu, W.Y.
[191-24-2]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of benzo[ghi]perylene to be 0.00026 mg(l) dm ⁻³ sln and $x_1$	
The corresponding mass percent calcu is 2.6 x 10 ⁻⁸ g(1)/100 g sln.	lated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL	<ol> <li>Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.</li> <li>doubly distilled.</li> </ol>
extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American	
Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. $\pm 10^{-5}$ mg(l) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Benzo[ghi]perylene; C₂₂H₁₂; [191-24-2]</pre>	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.	
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11, 133-6.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M. Kleinschmidt and D. Shaw	
Salinity: 6 g/kg sln (ref. 1)		
	······································	
EXPERIMENTAL VALUES:		
The solubility of benzo[ghi]perylene to be 0.21 $\mu\text{g/L}$ .	in salt water was reported	
The corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are 2.1 $\times 10^{-8}$ g(1)/100 g sln and 1.4 $\times 10^{-11}$ assuming a solution density of 1.004 kg/L.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
<pre>1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was cen- trifuged twice at 7000 g to remove suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma- tography. Spectrometric analysis of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.</pre>	Not given.	

	533
COMPONENTS :	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Benzo[b]triphenylene; C₂₂H₁₄;</li> <li>[215-58-7]</li> <li>(2) Salt Water</li> </ul>	<pre>Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. Khim. Tverd. Topl. <u>1977</u>, 11, 133-6.</pre>
NADTADI EC.	DEPADED NV.
VARIABLES: One temperature: 25°C Salinity: 6 g/kg sln (ref. 1)	PREPARED BY: M. Kleinschmidt and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of benzo[b]triphenyle to be 27.84 $\mu$ g/L.	ne in salt water was reported
The corresponding mass percent and m by the compilers are 2.719 x 10 ⁻⁶ g( assuming a solution density of 1.004	$1)/100 \text{ g sln and } 1.841 \times 10^{-9}$
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
<pre>1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was cen- trifuged twice at 7000 g to remove suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma- tography. Spectrometric analysis of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.</pre>	ESTIMATED ERROR:

COMPONENTS:	EVALUATOR:
<pre>(1) Dibenz[a,h]anthracene; C₂₂H₁₄; [58-70-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

#### CRITICAL EVALUATION:

Quantitative solubility data for dibenz[a,h]anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data are available for the solubility of water in dibenz[a,h]anthracene.

# TABLE 1. Quantitative Solubility Studies ofDibenz[a,h]anthracene (1) in Water (2)

······································		
Reference	Т/К	Method
Davis et al. (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. The two reported values, although obtained at slightly different temperatures, are in excellent agreement. Nevertheless there are insufficient data and the system is insufficiently well-characterized to justify a higher than Tentative classification.

# TABLE 2.Tentative Solubility Values ofDibenz[a,h]anthracene (1) in Water (2)

T/K		Solubility values	
	Reported values	"Best" val	
	10 ⁸ g(1)/100 g sln	10 ⁸ g(1)/100 g sln	10 ¹¹ <i>x</i> 1
298	5.84 (ref 2)	6	4
300	5 (ref 1)	5	3

#### REFERENCES

 Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.

2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98.

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Components :	ORIGINAL MEASUREMENTS:
(1) Dibenz[a,h]anthracene; C ₂₂ H ₁₄ ; [58-70-3]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc, <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
was reported to be 5 x $10^{-7}$ g(1) L ⁻¹ (Two identical results have been obta With the assumption that 1.00 L slr mass percent and mole fraction, $x_1$ , c 5 x $10^{-8}$ g(1)/100 g sln and 3 x $10^{-11}$	ined) $n \approx 1.00$ kg sln, the corresponding calculated by the compiler are
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in	<pre>SOURCE AND PURITY OF MATERIALS: (1) Eastman Kodak Company; purified; m.p. range 266.6-266.9°C or Hoffman La Roche; m.p. range 262.7-264°C (cf. ref 2).</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Dibenz[a,h]anthracene; C₂₂H₁₄; [58-70-3] (2) Water; H₂O; [7732-18-5]</pre>	Klevens, H.B. J. Phys. Chem. <u>1950</u> , 54, 283-98.	
VARIABLES:	PREPARED BY:	
Temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of dibenz[a,h]anthracene in water at 25°C was reported to be 2.15 x $10^{-9}$ mol(1) L ⁻¹ sln. With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are 5.84 x $10^{-8}$ g(1)/100 g sln and 3.88 x $10^{-11}$ .		
AUXILIARY	INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
The solubility of (1) in (2) was	(1) not specified.	
determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	(2) not specified.	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Dibenz[a,h]anthracene; C₂₂H₁₄; [53-70-3]</pre>	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.	
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11, 133-6.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M. Kleinschmidt and D. Shaw	
Salinity: 6 g/kg sln (ref. 1)		
EXPERIMENTAL VALUES:		
The solubility of dibenz[a,h]anthracene in salt water was reported to be 21.13 µg/L.		
The corresponding mass percent and mo by the compilers are 2.064 x 10 ⁻⁶ g(1 assuming a solution density of 1.004	$1)/100 \text{ g sln and } 1.397 \times 10^{-9}$	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
1L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was cen- trifuged twice at 7000 g to remove suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma-		
	ESTIMATED ERROR: temp. ± 1°C soly. ± 1.14 type of error not specified	
tography. Spectrometric analysis of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.	REFERENCES: 1. Krasnoshchekova, R.Ya; Guber- grits, M.Ya. Neftekhimiya 1973, 13, 885.	

COMPONENTS :	ORIGINAL MEASUREMENTS:
	OKTOINE PERSONERENIS:
(1) Dibenz[a,j]anthracene; C ₂₂ H ₁₄ ; [224-41-9]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of dibenz[a	a,j]anthracene in water
t/°C	$10^{5}$ g(1) L ⁻¹ (2)
27	1.1 $\pm$ 0.1 1.0 $\pm$ 0.2 1.3 $\pm$ 0.2
With the assumption that 1.00 L slm mass percent and mole fraction, $x_1$ , c 1.2 x $10^{-6}$ g(1)/100 g sln and 7.8 x J	calculated by the compiler are
AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:

	ORIGINAL MEASUREMENTS:	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Dibenz[a,j]anthracene; C₂₂H₁₄; [224-41-9]</pre>	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.	
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11, 133-6.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C Salinity: 6 g/kg sln (ref. 1)	M. Kleinschmidt and D. Shaw	
EXPERIMENTAL VALUES:	I	
EXPERIMENTAL VALUES:		
The solubility of dibenz[a,j]anthrac to be 10.544 µg/L.	cene in salt water was reported	
The corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are 1.029 x $10^{-6}$ g(1)/100 g sln and 6.970 x $10^{-10}$ assuming a solution density of 1.004 kg/L.		
AUXILIARY	INFORMATION	
METHOD / APPARATUS / PROCEDURE :		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
<pre>1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the ace- tone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried resi- due, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis.</pre>		
The solution was centrifuged twice at 7000 g to remove suspended par-	ESTIMATED ERROR:	
ticles. The hydrocarbon was ex-	temp. ± 1°C	
tracted with benzene and concen- trated by evaporation, then purified	soly. ± 1.05 type of error not specified	
using thin-layer chromatography. Spectrometric analysis of an octane	REFERENCES :	
solution of the hydrocarbon was done using the quasilinear lumi- nescence spectra.	<ol> <li>Krasnoshchekova, R.Ya; Guber- grits, M.Ya. Neftekhimiya 1973, 13, 885.</li> </ol>	

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 COMPONENTS:
 ORIGINAL MEASUREMENTS:

 (1) Picene; C<sub>22</sub>H<sub>14</sub>; [213-46-7]
 Davis, W.W.; Krahl, M.E.;
Cloves, G.H.A.

 (2) Water; H<sub>2</sub>O; [7732-18-5]
 J. Am. Chem. Soc. <u>1942</u>, 64,
108-10.

 VARIABLES:
 PREPARED BY:

 One temperature: 27°C
 M.C. Haulait-Pirson
```

EXPERIMENTAL VALUES:

The solubility of picene in water at 27°C was reported to be 2.5 x 10⁻⁶ g(1) L⁻¹ (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 2.5 x 10⁻⁷ g(1)/100 g sln and 1.6 x 10⁻¹⁰.

AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	<pre>INFORMATION SOURCE AND FURITY OF MATERIALS: (1) prepared at the Ohio State University; m.p. range 363.5-364.5°C; (cf. ref 2). (2) dust-free.</pre>
	ESTIMATED ERROR: temp. ± 3°C soly. ± 0.5 x 10 ⁻⁶ g(1) dm ⁻³ (2) REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. <u>1942</u> , 64, 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1940</u> , 62, 3086.

COMPONENTS :	
	ORIGINAL MEASUREMENTS:
<pre>(1) 10-Butylbenz[a]anthracene; C₂₂H₂₀; [31632-63-0]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of 10-butylbe	nz[a]anthracene in water
t/°C	$10^6$ g(1) L ⁻¹ (2)
27	7 ± 0.7 7 ± 0.7 7 ± 0.7 8 ± 1 8 ± 1
8.0 x $10^{-7}$ g(l)/100 g sln and 5.1 x l	
	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:

COMPONENTS :	ORIGINAL MEASUREMENTS:	
<pre>(1) 7-Pentylbenz[a]anthracene; C₂₃H₂₂; [63019-00-1]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.	
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.	
VARIABLES:	PREPARED BY:	
One temperature: 27°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:	4	
Solubility of 10-penthy	benz[a]anthracene in water	
<i>t/°C</i>	$10^7 g(1) L^{-1} (2)$	
27	9 ± 1	
	8 ± 3	
	8 ± 2	
mass percent and mole fraction, $x_1$ , 8 x 10 ⁻⁸ g(1)/100 g sln and 5 x 10 ⁻¹	calculated by the compiler are !	
AUXILIARY	INFORMATION	
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	<ul> <li>(1) prepared at Harvard University; m.p. range 82.6-83.3°C (cf. ref 2).</li> <li>(2) dust-free.</li> <li>(2) dust-free.</li> <li>ESTIMATED ERROR: temp. ± 3°C soly. see above</li> <li>REFERENCES:</li> <li>1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101.</li> <li>2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940,</li> </ul>	

COMPONENTS: (1) Coronene; C ₂₄ H ₁₂ ; [191-07-1]	ORIGINAL MEASUREMENTS: Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of coronene in water to be 0.00014 mg(1) dm ⁻³ sln and $x_1$ . The corresponding mass percent calcu	$= 8.56 \times 10^{-12}$ .
is $1.4 \times 10^{-8}$ g(1)/100 g sln.	lated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.</li> <li>(2) doubly distilled.</li> </ul>
Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. $\pm 2 \times 10^{-5}$ mg(1) dm ⁻³ sln (maximum deviation from several
	determinations).

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1)	
(1) Hexacosane; C ₂₆ H ₅₄ ; [110-82-7]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES:	PREPARED BY:
One temperatures 25°C	M.C. Haulait-Pirson
One temperature: 25°C	M.C. Haulalt-Filson
EXPERIMENTAL VALUES:	
The solubility of hexacosane in water	
$1.7 \times 10^{-7} g(1)/100 g(2)$ correspondin 0.8 x 10 ⁻¹⁰ .	ig to a mole fraction $x_1$ , of
0.8 x 10 .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
175 mg (1) were equilibrated with	(1) Analabs Inc., 99+%.
700 mL (2) in closed flasks by sha- king on a constant temperature bath	(2) doubly distilled.
for 12 hours. The flasks were then	
allowed to stand for 24 hours. Aliquots of 100 mL were removed,	
filtered through a 0.45 µm Millipore filter, then extracted three times	
with 10-mL portions of hexane con- taining an internal standard. The	
concentration of (1) was determined	ESTIMATED ERROR:
by injection of the hexane extract into a dual column gas chromatograph	
equipped with flame ionization de- tectors.	temp. ± 0.1°C soly. ± 16%
	REFERENCES :
1	1

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Components :	ORIGINAL MEASUREMENTS:
(1) Hexacosane; C ₂₆ H ₅₄ ; [630-01-3] (2) Seawater	Sutton, C.; Calder, J.A.
(2) Seawater	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C One salinity: 35 g salts/kg sln	P.A. Meyers and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of hexacosane in seawa $1 \times 10^{-8} \text{ g(1)/100 g sln and } x_1 = 6 \times 10^{-8} \text{ g(1)/100 g sln}$	
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The com- ponents were equilibrated by gentle shaking for 12 hrs at $25.0 \pm 0.1^{\circ}$ C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 µm membrane filters to remove any hydrocarbon droplets. The filtrate was extrac- ted three times with hexane and ana- lyzed by gas chromatography.	<ul> <li>Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons.</li> <li>Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</li> <li>ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.</li> </ul>

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ORIGINAL MEASUREMENTS:
COMPONENTS:
 Baker, E.G.
 (1) Hexatriacontane; C<sub>36</sub>H<sub>74</sub>;
 [630-06-8]
 Am. Chem. Soc., Div. Petrol.
 Chem., Preprints 1958, 3, N°4,
 (2) Water; H<sub>2</sub>O; [7732-18-5]
 C61-8.
VARIABLES:
 PREPARED BY:
 M.C. Haulait-Pirson
One temperature: 25°C
EXPERIMENTAL VALUES:
The solubility of hexatriacontane-18,19-C<sup>14</sup> in water at 25°C was
 reported to be 1.7 \times 10^{-9} q(1)/q(2).
The corresponding mass percent and mole fraction, x_1, calculated by
the compiler are 1.7 \times 10^{-7} \text{ g(1)}/100 \text{ g sln and } 6.1 \times 10^{-11}.
 AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:
 SOURCE AND PURITY OF MATERIALS:
 (1) New England Nuclear Corporation;
 Carbon-14 labeled (1) was used
 used as received.
 as tracer.
 The technique of preparing a satu-
 (2) distilled.
 rated aqueous solution of (1) by
 ultrafiltration of a (1)-(2) dis-
 persion has been described in ref 1.
 A Packard Tri-Carb Liquid Scintilla-
 tion Spectrometer was used to detect
 the radioactive (1) dissolved in
 (2).
 ESTIMATED ERROR:
 soly. 20% (standard deviation from
 17 replicate runs).
 REFERENCES:
 1. Baker, E.G. Am. Chem. Soc.
Div. Petrol. Chem., Preprints-
 Symposia 1956, 1, N°2, 5.
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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Hexatriacontane; C ₃₆ H ₇₄ ; [630-06-8]	Baker, E.G.
	Science <u>1959</u> , 129, 871-4.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of hexatriacontane in	Wator at 25°C was reported
to be 2.09 x $10^{-7}$ mL (1)/100 mL (2).	water at 25 C was reported
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
not specified.	not specified.
not specified.	not spectred.
	ESTIMATED ERROR:
	not specified.
	DEFEDENCYC
	REFERENCES :

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