INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

ANALYTICAL CHEMISTRY DIVISION COMMISSION ON SOLUBILITY DATA

# **SOLUBILITY DATA SERIES**

.

Volume 49

# ESTERS WITH WATER PART II: ESTERS 7-C TO 32-C

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# SOLUBILITY DATA SERIES

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# SOLUBILITY DATA SERIES

Volume 49

# **ESTERS WITH WATER** PART II: ESTERS 7-C TO 32-C

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# FOREWORD

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

The Solubility Data Series is a project of Commission V.8 (Solubility Data) of the International Union of Pure and Applied Chemistry (IUPAC). The project had its origins in 1973, when the Analytical Chemistry Division of IUPAC set up a Subcommission on Solubility Data under the chairmanship of the late Prof. A. S. Kertes. When publication of the *Solubility Data Series* began in 1979, the Committee became a full commission of IUPAC, again under the chairmanship of Prof. Kertes, who also became Editor-in-Chief of the Series. The Series has as its goal the preparation of a comprehensive and critical compilation of data on solubilities in all physical systems, including gases, liquids and solids.

The motivation for the Series arose from the realization that, while solubility data are of importance in a wide range of fields in science and technology, the existing data had not been summarized in a form that was at the same time comprehensive and complete. Existing compilations of solubility data indeed existed, but they contained many errors, were in general uncritical, and were seriously out-of-date.

It was also realized that a new series of compilations of data gave educational opportunities, in that careful compilations of existing data could be used to demonstrate what constitutes data of high and lasting quality. As well, if the data were summarized in a sufficiently complete form, any individual could prepare his or her own evaluation, independently of the published evaluation. Thus, a special format was established for each volume, consisting of individual data sheets for each separate publication, and critical evaluations for each separate system, provided sufficient data from different sources were available for comparison. The compilations and, especially, the evaluation were to be prepared by active scientists who were either involved in producing new data, or were interested in using data of high quality. With minor modifications in format, this strategy has continued throughout the Series.

In the standard arrangement of each volume, the Critical Evaluation gives the following information:

(i) A text which discusses the numerical solubility information which has been abstracted from the primary sources in the form of compilation sheets. The text concerns primarily the quality of the data, after consideration of the purity of the materials and their characterization, the experimental method used, the uncertainties in the experimental values, the reproducibility, the agreement with accepted test values, and finally, the fitting of the data to suitable functions, along with statistical tests of the fitted data. (ii) A set of recommended data, whenever possible, including weighted averages and estimated standard deviations. If applicable, one or more smoothing equations which have been computed or verified by the evaluator are also given.

(iii) A graphical plot of the recommended data, in the form of phase diagrams where appropriate.

The Compilation part consists of data sheets which summarize the experimental data from the primary literature. Here much effort is put into obtaining complete coverage; many good data have appeared in publications from the late nineteenth and early twentieth centuries, or in obscure journals. Data of demonstrably low precision are not compiled, but are mentioned in the Critical Evaluation. Similarly, graphical data, given the uncertainty of accurate conversion to numerical values, are compiled only where no better data are available. The documentation of data of low precision can serve to alert researchers to areas where more work is needed.

A typical data sheet contains the following information:

- (i) list of components: names, formulas, Chemical Abstracts Registry Numbers;
- (ii) primary source of the data;
- (iii) experimental variables;
- (iv) compiler's name;
- (v) experimental values as they appear in the primary source, in modern units with explanations if appropriate;
- (vi) experimental methods used;
- (vii) apparatus and procédure used;
- (viii) source and purity of materials used;
  - (ix) estimated error, either from the primary source or estimated by the compiler;
  - (x) references relevant to the generation of the data cited in the primary source.

Each volume also contains a general introduction to the particular type of system, such as solubility of gases, of solids in liquids, etc., which contains a discussion of the nomenclature used, the principle of accurate determination of solubilities, and related thermodynamic principles. This general introduction is followed by a specific introduction to the subject matter of the volume itself.

The Series embodies a new approach to the presentation of numerical data, and the details continue to be influenced strongly by the perceived needs of prospective users. The approach used will, it is hoped, encourage attention to the quality of new published work, as authors become more aware that their work will attain permanence only if it meets the standards set out in these volumes. If the Series succeeds in this respect, even partially, the Solubility Data Commission will have justified the labour expended by many scientists throughout the world in its production.

January, 1989

J. W. Lorimer, London, Canada

# PREFACE

This volume, one of a pair in the Solubility Data Series devoted to esters in water, includes solubility data for binary systems containing an ester and water published up through the end of 1988. The first volume contains the esters having two through six carbon atoms with water and the second volume contains esters having seven or more carbon atoms with water. With only rare exceptions, the compiled data and evaluations involve measurements made at constant pressure over rather restricted ranges of temperature. The limited ranges of pressure and temperature involved are to be expected in view of the liquid-liquid condition prescribed for the systems.

For the most part, the data presented show general patterns of behavior expected for the topic systems. While rather extensive data have been reported for many of the systems under consideration, no effort was made to attempt any detailed correlations of behavior or descriptions of trends beyond those presented by the evaluator in the evaluation sections.

The critical evaluations were all prepared by one author and an introductory section has been included to elaborate the philosophy and methodology followed in the evaluations. No attempts were made to extract thermodynamic parameters such as activity coefficients, enthalpies of solution, and the like from the reported data although much of the published work is sufficiently precise for such activities.

Every attempt was made to include all published data for the subject systems through the end of 1988. The editors would be grateful for any information concerning material which was overlooked in the preparation of this work.

The editors would like to express their appreciation to all those who have provided assistance in the volume preparation, especially to fellow members of the IUPAC Commission on Solubility Data and to those who have served as reviewers of this work.

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November 1991.

LIQUID-LIQUID SOLUBILITY: EVALUATION PHILOSOPHY AND METHODOLOGY

G.T. HEFTER

### INTRODUCTION

Because of the differing ways in which it is possible to critically evaluate published solubility data it is worthwhile to present a coherent statement on the philosophy and procedures which have been used in this volume. Although this is a personal statement concerning the present volume, many of the ideas have been developed by myself as an evaluator for previous liquid-liquid volumes in the Solubility Data Series [1-3] and are shared, to some degree, by other evaluators.

# EVALUATION PHILOSOPHY

The critical evaluation of data is, at least in part, a subjective process. Some physical scientists are uncomfortable with this notion but the history of science shows us it is undeniable. Because some subjective judgements are inevitably involved, it is vital that the evaluator's procedure should be as visible as possible. In this way, if the user does not agree with the evaluator's judgement or arguments or if new data become available it is possible, with a minimum of effort, to derive a new set of preferred or "best" values. For this reason the Critical Evaluations in this and those previous volumes to which I have contributed [1-3] have been, in essence, written like research papers with enough information provided for users to repeat or change the evaluation should they so desire.

The starting point for each Critical Evaluation is that the data compilation is complete, i.e., the data sheets include all the available data. This is an important premise because the addition of extra data may change the evaluation considerably. This is especially true of liquid-liquid systems since very few have been adequately studied over a wide temperature range and disagreements often exist between independent investigations.

In general, a "democracy of observers" is followed. That is, the data of all investigators are given equal weight irrespective of their reputation or location. This is justifiable in scientific terms because experience shows that real "errors" in liquid-liquid solubility data are much greater than individual authors' reported precisions. Thus, the benzene-water system, which is relatively simple and probably the most widely studied of all liquid-liquid systems [2], has solubilities which are known to an accuracy of about  $\pm 2$ % (relative). The same estimated error is obtained regardless of whether a simple average of the available data is taken or whether a complex weighting procedure is used. This suggests that, at the present stage of development of liquid-liquid solubility determinations, equal weighting for all data is the most appropriate course of action. The exceptions to this rule are discussed below.

### **REJECTION OF DATA**

The statement that all data are given equal weight must be qualified: some data are assigned zero weight, i.e., they are rejected. Data rejection is potentially dangerous, especially when few data are available. Nevertheless, since a critical evaluation is required, it has to be considered. The most important reasons for rejecting data are as follows.

1. The data disagree "significantly" from most other studies (especially if these are numerous). Significance is subjective but a criterion of

 $| \mathbf{s}_{obs} - \mathbf{s}_{av} | > 3\sigma_n$ 

- where s<sub>obs</sub> is the reported solubility datum being considered for rejection
  - s<sub>av</sub> is the arithmetic average (mean) of all other studies at the same temperature and pressure
  - $\sigma_n$  is the standard deviation from the mean of these studies

has been generally, but not rigidly, applied [1-3].

It should be noted that this procedure can be invoked only once. That is, having rejected some points in a particular data set it is not statistically valid to recalculate a new value of  $\sigma_n$  and then reject further points. Strictly speaking this means that outlying data should be included in the original calculation of  $\sigma_n$ . However, the amount of available data does not always make this approach realistic and common sense must be applied.

- 2. Approximate data (one significant figure) are rejected when a reasonable amount of more precise data is available.
- 3. Data which are grossly inconsistent with chemical systematics or thermodynamic expectations are also rejected.
- 4. In keeping with the practice adopted in previous liquid-liquid solubility values, data originally presented in graphical form or in volume ratio units are also excluded. In the latter case, data are retained if appropriate density data are readily available to permit conversion to mass units. As density measurements are usually far more reliable than solubility data, the choice of density values is usually not critical.

It is appropriate to add here that data for a particular system coming from the same authors or the same laboratories have generally not been regarded as independent measurements and have therefore been subsumed into a single result (at each temperature).

### THE EVALUATION FORMAT

The Critical Evaluations in this volume follow the format evolved in previous liquid-liquid solubility volumes [1-3]. In essence each Evaluation is divided into three parts. In the first part Table 1 lists all the available publications containing quantitative solubility data for the particular system. Broad experimental details such as temperature range, type of solubility measured ((1) in (2), (2) in (1) or mutual) and the method used are also included in Table 1. After mention of any other special features such as critical points, or any special types of investigation, further discussion is usually divided into two parts: the solubility of the organic in the aqueous phase, and that of water in the organic-rich phase. Since these two sections are handled in the same way they will be discussed together.

After listing rejected data, anomalies and caveats, all the available data (usually expressed as g/100g sln) are collected into Tables (usually Tables 2 & 3). To facilitate comparisons, data are interpolated (if necessary) to specific temperatures at 5K intervals near 298K, then 10 or 20K intervals. These temperatures are exact, i.e. 298.15, 303.15 ... K but for convenience are written 298, 303, ... K in the text. The nature of most liquid-liquid solubility data makes graphical interpolated with an asterisk (\*). Very occasionally data are extrapolated but only over a short range (<5K) and only if the solubility curve is not changing sharply.

All the retained values at each temperature are then averaged and the mean and  $\sigma_n$  recorded in the Tables. Few of the systems in this volume have sufficient data to permit meaningful statistical analysis. The value of  $\sigma_n$  is therefore included only as a convenient measure of the spread of the experimental data.

#### "BEST" VALUES

The word "best", almost always in inverted commas (quotation marks), is used throughout the Critical Evaluations in this and previous liquid-liquid solubility volumes [1-3] in a specific way: to mean "best available estimate". It follows from what has been said above that "best" values are simply the arithmetic average (mean) of all the accepted data, including those obtained by interpolation and excluding rejected data. "Best" values are given in both g/100g sln and mole fraction units (x).

#### **RECOMMENDED VALUES**

Solubilities are recommended only if two or more independent studies (including rejected data) agree to within  $\pm$  5%(relative), i.e.,

 $|100\sigma_n/s_{av}| \leq 5$ 

and there are no other obvious problems. Recommended data are designated by (R) immediately following the numerical value.

For sparingly soluble systems this criterion may be too harsh and

 $| 100\sigma_{\rm n}/s_{\rm av} | \le 10 \text{ or } 20$ 

may be more appropriate [3]. Very few high molecular weight esters have been sufficiently well characterized to enable even these less restrictive criteria to be applied.

Data which are not "Recommended" are regarded as "Tentative". The likely accuracy of these data varies from system to system and from temperature to temperature but may be inferred from

1. σ<sub>n</sub>

2.  $100\sigma_{\rm n}/s_{\rm av}$ 

3. n (the number of independent measurements).

Occasionally there are definite reasons to suspect the available data are not reliable. Such data are labelled "Doubtful" and the detailed reasons for this classification given. Considerable care should be exercised in the use of such data.

Note that the mole fraction "best" solubilities in each table should be regarded as having the same status ("Recommended", "Tentative" or "Doubt-ful") and the same (relative) percentage uncertainties (where given) as the corresponding mass % solubilities.

#### GRAPHICS

In systems for which a reasonable amount of data exists, selected results are plotted graphically over the studied temperature range. Appropriate comments on the plots are made in the figure caption or in the text.

## FITTING EQUATIONS

The use of fitting equations to smooth solubility data as a function of temperature is controversial and a topic in its own right which will not be discussed here. As in previous liquid-liquid solubility volumes [1-3], fitting equations are not generally given in the printed version of this volume. There are several reasons for this.

- 1. There is no single equation form which can be used for all systems.
- The data for some systems are too scattered or poorly defined for realistic curve fitting.
- 3. Without special care empirical fitting equations may give misleading results (spurious extrema, etc.) when interpolating and can almost never be reliably used for extrapolation.

For certain systems where reliable data appear evident, fitting equations have been provided. Such equations come directly from the original works or from the efforts of the compilers in the course of their examination of reported data and preparation of smoothed value tables.

Users who wish to derive their own fitting equations are advised to do so with caution. It is suggested that the "best" values be used for this purpose, but it should be noted that this may create anomalies because of the Way in which the "best" values are derived (see above). Where fitting equations are given in this volume they should be used only over the stated range.

#### THERMODYNAMIC CONSISTENCY

Using standard relationships from thermodynamics it can be shown that:

$$\frac{\partial (\Delta_{gln} G/T)}{\partial T} = - \frac{\Delta_{gln} H}{RT^2}$$

 $\Delta_{sln}G = -RT \ln a_{sat}$ 

and

 $\frac{\partial^2 (\Delta_{sln} G/T)}{\partial T^2} = \frac{\partial (\Delta_{sln} H)}{\partial T} = \Delta_{sln} C_p$ 

where  $\Delta_{gln}G$ ,  $\Delta_{gln}H$  and  $\Delta_{gln}C_p$  are respectively the Gibbs energy, enthalpy and heat capacity (at constant pressure) changes corresponding to the dissolution of the solute in the solvent and  $a_{gat}$  is the activity of the saturated solute in the solvent. If the solute is only sparingly soluble the thermodynamic parameters may be equated with their standard state values, and it should be noted that  $\Delta_{gln}C_p$  may itself be temperature dependent.

Both  $\Lambda_{gln}H$  and  $\Lambda_{gln}C_p$ , at least in principle, can be measured directly by separate calorimetric procedures [5,6] and therefore can serve as an independent check on the temperature dependence of published solubility data. This approach has been used with significant effect in evaluating hydrocarbon solubilities in water [2-3]. However, very few calorimetric data have been reported for ester-water systems and so this approach has not been utilized in the present volume.

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- 5. S.O. Nilsson and I. Wadso, J. Chem. Thermodyn. 1984, 16, 317.
- 6. P. Picker, P.A. Leduc, P.R. Philip and J.E. Desnoyers, J. Chem. Thermodyn. 7, 3, 641.

	1
COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul><li>(1) 2-Propenoic acid, 2-methyl-,</li><li>2-cyanoethyl ester</li></ul>	Frolov, A.F.; Maiorova, N.M.; Erykov, V.G.; Korshukov, M.A.
(2-cyanoethyl methacrylate); C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub> ; [4513-53-5]	Zh. Prikl. Khim. <u>1977</u> , 50, 1318-21.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of 2-methyl-2-propending $20^{\circ}$ C was reported to be 1.7 g(1)/100g tion, x <sub>1</sub> , value calculated by the cont	ic acid 2-cyanoethyl ester in water at sln. The corresponding mole frac- piler is 0.0022.
	· · · · · · · · · · · · · · · · · · ·
The solubility of water in 2-methyl-2 20 <sup>o</sup> C was reported to be 2.9 g(2)/100g tion, $x_2$ , value calculated by the com	2-propenoic acid 2-cyanoethyl ester at f sln. The corresponding mole frac- apiler is 0.19.
,	
AUXILIARI	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified; b.p. 240.0°C, d <sub>4</sub> <sup>20</sup> 1.0400, n <sub>D</sub> <sup>20</sup> 1.4460.
	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

2				
COMPONENT	S:		ORIGINAL MEASUREM	ENTS:
(1) Formic acid cyclohexyl ester			Stephenson, R.;	Stuart, J.
( <i>cy</i> [43	clohexyl format 51-54-6]	); C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> ;	J. Chem. Eng. Da 56-70.	ta <u>1986</u> , 31,
(2) Wat	er; H <sub>2</sub> O; [7732-:	L8-5]		
VARIABLES	:		PREPARED BY:	
T/K = 27	3 - 363		Z. Maczynska	
EXPERIMEN	TAL VALUES:			
Mu	tual solubility	of formic aci	d cyclohexyl ester	and water
t/°C	g(1)/10	)0g sln	$x_1$ (com	piler)
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	e (1)-rich phase
0		98.90		0.9267
9.3	1.70	98.58	0.00242	0.9070
19.0	0.65	98.44	0.00092	0.8987
29.6	0.39	98.63	0.00055	0.9101
39.5	-	98.61	-	0.9088
49.9	-	98.36	-	0.8939
69.9	-	98.10	-	0.8789
80.0	-	97.87	-	0.8659
90.3	-	97.50	-	0.8457
std. dev. 0.01 0.02				
		AUXILIARY 1	INFORMATION	
METHOD/AP	PARATUS/PROCEDU	RE:	SOURCE AND PURITY	OF MATERIALS:
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.		<ul> <li>(1) Source not s</li> <li>cial sample;</li> <li>as received.</li> <li>(2) Not specifie</li> </ul>	pecified, commer- purity 95%; used	
		(2) NOU Specifie	u.	
		ESTIMATED ERROR: Accuracy of meth for solubility,	od 0.1 wt% or less, see above.	
		REFERENCES:		

		3
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ul> <li>(1) 2-Propenoic acid butyl ester</li> <li>(butyl acrylate); C<sub>7</sub>H<sub>12</sub>O<sub>2</sub>;</li> <li>[141-32-2]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	Logutov, V.I.; Danov, S.M.; Chubarov, G.A.; Tomashchuk, V.I. Zh. Prikl. Khim. <u>1983</u> , 56(1), 214-6.	
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of 2-Propenoic acid butyl ester in water at 20°C was reported to be 0.18 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calculated by the compiler is 2.6 x 10 <sup>-4</sup> . The solubility of water in 2-Propenoic acid butyl ester at 20°C was reported to be 0.65 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calculated by the compiler is 0.044. The densities of the water-rich phase and the ester rich phase were reported to be $d_{20}^{20}$ 0.9981 and $d_{20}^{20}$ 0.8987 respectively.		
AUXILIARY :	(NFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The analytical method was used. After mixing and separating, the two samples were analysed. The water in organic phase was deter- mined by titration with Karl Fischer reagent. The 2-Propenoic acid butyl ester was measured by the gas-liquid chromatography	(1) Source not specified; used as received; b.p. 147.4°C, $d_4^{20}$ 0.9010, $n_D^{20}$ 1.4200. (2) Twice distilled.	
method with an inert standard or by the bromate titration method. Both	ESTIMATED ERROR:	
procedures gave similar results.	Temp. ±0.5°C. Soly. ±(2-3)% (relative) (2) in organic phase, ±3% (relative) (1) in water phase.	
	REFERENCES:	

4		
COMPONENTS: (1) Propanedicic acid diethyl	ORIGINAL MEASUREMENTS: Sobotka, H.; Kahn, J.	
ester (diethyl malonate); C <sub>7</sub> H <sub>12</sub> O <sub>4</sub> ; [105-53-3]	J. Am. Chem. Soc. <u>1931</u> , 53, 2935-8.	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of propanedioic acid diethyl ester in water at 20°C was reported to be 2.08 g(1)/100mL(2). The corresponding mass per cent and mole fraction, $x_1$ , values calculated by the compiler are 2.04 g(1)/100g sln and 0.0023. Density of water $d_4^{20} = 0.9982$ (ref 1) was used in the calculation.		
	TNFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent droplets.	<ul> <li>(1) Source not specified (Eastman Kodak Laboratories or synthe- sized); twice-distilled under reduced pressure; d<sup>20</sup><sub>4</sub> 1.0550, n<sup>20</sup><sub>D</sub> 1.4144.</li> <li>(2) Distilled.</li> <li>ESTIMATED ERROR: Not specified.</li> <li>REFERENCES:</li> <li>1. Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Towas A and M University Towas</li> </ul>	

COMPONENTS:			ORTGINAL MEASUREMENTS:		
(1) Pertonadicia anid direthul			ORIGINAL MEASUREMENTS:		
(1) Pentanedioic acid dimethyl ester (dimethyl glutarate):			Stephenson, R.; Stuart, J.		
$C_{2}H_{12}O_{4}$ ; [1119-40-0]			J. Chem. Eng. Da: 56-70.	ta <u>1986</u> , 31,	
(2) Wat	$er; H_2O; [7732-1]$	- 18-5]			
VARIABLES	;		PREPARED BY:		
T/K = 27	3 - 364		Z. Maczynska		
				•	
EXPERIMEN Mutu	TAL VALUES: al solubility of	f pentanedioic	acid dimethyl est	er and water	
t/°c	α(1)/1(		X. (COM)	piler)	
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase	
0	7.1	97.70	0.0085	0.8269	
9.4	6.3	97.37	0.0075	0.8063	
20.0	6.1	97.72	0.0072	0.8282	
29.6	5.9	96.44	0.0070	0.7529	
39.5	5.8	95.88	0.0069	0.7236	
49.8	5.8	95.36	0.0069	0.6980	
60.3	6.1	94.69	0.0072	0.6673	
70.2	6.4	92.89	0.0076	0.5950	
80.0	6.6	92.86	0.0079	0.5939	
90.5	8.1	91.77	0.0098	0.5564	
std. d	ev. 0.10	, 0.03		<u></u>	
		AUXILIARY I	NFORMATION		
METHOD/AP	PARATUS/PROCEDU	RE:	SOURCE AND PURITY	OF MATERIALS:	
The anal	ytical method wa	s used.	(1) Source not specified, commer- cial sample; purity 98%; used		
Componen With com	t (1) was equili	brated			
temperat	ure in a thermos	stat. Each			
layer was	s sampled with a determined by ad	syringe;	(2) Not specified	1.	
weighed amount of acetonitrile					
(or sometimes propanol) to the organic layer sample and measuring				······································	
by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).			ESTIMATED ERROR:		
			Accuracy of method 0.1 wt% or less,		
			for solubility, s	see above.	
boiling material (e.g. 1-hexanol)					
Was used to determine (2) in the					
Leer ra	7.7. •		REFERENCES:		
		1			

COMPONENTS:	EVALUATOR:
(1) Acetic acid 1-methyl-1-butyl ester (1-methylbutyl acetate) $C_7H_{14}O_2$ ; [626-38-0]	G.T. Hefter, School of Mathematical ; and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H <sub>2</sub> O; [7732-18-5]	January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid 1-methyl-1-butyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>TABLE 1: Quantitative Solubility Studies of the</u> Acetic acid 1-methyl-1-butyl ester (1) - Water (2) System			
Reference	T/K	Solubility	Method
Park and Hopkins (ref 1)	298	(1) in (2)	unspecified
Doolittle (ref 2)	293	mutual	unspecified

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

As can be seen from Table 1 no data have been reported under comparable conditions and so no Critical Evaluation is possible. Furthermore, the datum of Park and Hopkins (ref 1) is reported only in v/v units and would normally be excluded from consideration. However, assuming a density of 0.86 g/mL for (1) (ref 2) and a density of 1.00 g/mL for the saturated solution of (1) in (2), the solubility reported by Park and Hopkins (ref 1) at 298 K is equivalent to 0.23 g(1)/100 g sln which is in good agreement with Doolittle's value of 0.19 g(1)/100 g sln at 293 K (ref 1). Doolittle (ref 1) also reports a value of 0.88 g(2)/100 g sln for the solubility of water in the ester. The interested user is referred to the relevant Data Sheets for additional information.

REFERENCES

Park, J. G.; Hopkins, M. B. Ind. Eng. Chem. <u>1930</u>, 22, 826-30.
 Doolittle, A. K. Ind. Eng. Chem. <u>1935</u>, 27, 1169-79.

COMPONENTIC	ODICINAL MEACUDEMENTS-
COMPONENTS:	Deck I G & Werking N D
(1) Acetic acid 1-methyl-1-butyl ester (1-methylbutyl acetate);	Park, J.G.; Hopkins, M.B.
$C_7H_{14}O_2$ ; [626-38-0]	Ind. Eng. Chem. <u>1930</u> , 22, 826-30.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of acetic acid 1-methy reported to be 0.2 mL(1)/100mL(2).	l-1-butyl ester in water at 25°C was
AUXILIARY I	NFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	<ul> <li>(1) Source not specified, commercial samples; used as received; 85-88% of ester, b.p. range 128-134°C.</li> <li>(2) Not specified.</li> </ul>
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

,

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid 1-methyl-1-butyl	Doolittle, A.K.	
ester (1-methylbutyl acetate);	Ind. End. Chem. <u>1935</u> , 27, 1169-79.	
$C_7 n_{14} O_2$ ; [626-38-0]		
(2) water; $H_20$ ; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
FYDEDIMENTAL VALUES.	L	
EXPERIMENTAL VALUES: The solubility of acetic acid 1-methyl-1-butyl ester in water at $20^{\circ}$ C was		
reported to be 0.19 g(1)/100g sln. Th	The corresponding mole fraction, $x_1$ ,	
value calculated by the compiler is 2	$1.6 \times 10^{-4}$ .	
The solubility of water in acetic aci	d 1-methyl-1-butyl ester at 20°C was	
reported to be 0.88 $g(2)/100g sin$ . The value calculated by the compiler is 0	le corresponding mole fraction, $x_2$ ,	
value calculated by the compiler is t		
AUXILIARY 1	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Source not specified,	
	commercial product; purity 92%, b.p. range $121-144$ °C, $d_4^{20}$ 0.862.	
	(2) Not specified	
	ESTIMATED ERROR:	
	Not specified.	
	-	
	DEFEDENCES.	
	ALF ERENCED ;	

Сомро	NENTS:	EVALUATOR:
(1)	Acetic acid 3-methyl-1-butyl ester ( <i>isopentyl acetate</i> ); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [123-92-2]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia January, 1989

#### CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid 3-methyl-1-butyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>Acetic acid 3-methyl-1-butyl ester (1) - Water (2) System</u>			
Reference	т/к	Solubility	Method
Bancroft (ref 1)	293	mutual	titration
Othmer et al. (ref 2)	297	mutual	unspecified
Narasimhan <i>et al</i> . (ref 3)	303	mutual	titration, refractometric
Iguchi and Fuse (ref 4)	298	mutual	titration
Ramanarao <i>et al</i> . (ref 5)	303	mutual	turbidometric
Andreeva et al. (ref 6)	367	mutual	titration
Rao et al. (ref 7)	303	mutual	titration
Skrzecz (ref 8)	288-359	mutual	synthetic, Karl Fischer
Stephenson and Stuart (ref 9)	273-364	mutual	GLC

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. SOLUBILITY OF ACETIC ACID 3-METHYL-1-BUTYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid 3-methyl-1butyl ester (1) in water (2) are summaized in Table 2 with the following exceptions.

The value of Bancroft (ref 1) reported in v/v units is excluded from consideration. The data reported by Iguchi and Fuse (ref 4), Ramanarao et al. (ref 5) and Andreeva et al., (ref 6) are substantially higher (>  $3\sigma_n$ ) than other values and have been rejected. The datum of Othmer et al. (ref 2), which is considerably lower than other studies is also rejected.

(continued next page)

сомро	NENTS:	EVALUATOR:
(1)	Acetic acid 3-methyl-1-butyl	G.T. Hefter, School of Mathematical
	ester (isopentyl acetate);	and Physical Sciences,
	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [123-92-2]	Murdoch University, Perth, W.A.,
(2) Wat	Water: H_O: [7732-18-5]	Australia
		January, 1989

CRITICAL EVALUATION: (continued)

The remaining data, largely due to Skrzecz (ref 8) and Stephenson and Stuart (ref 9) are in excellent agreement, enabling the average "Best" values to be Recommended over a wide temperature range. Selected data are plotted in Figure 1.

> TABLE 2: Recommended (R) and Tentative Solubilities of Acetic acid 3-methyl-1-butyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm \sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln $10^4 x_1$	
273	0.34 (ref 9)	0.34 4.7	
283	0.260 <sup>*</sup> (ref 9)	0.26 3.6	
293	0.218 <sup>*</sup> (ref 8), 0.220 <sup>*</sup> (ref 9)	0.219 ± 0.001 (R) 3.03	
298	0.207 <sup>*</sup> (ref 8), 0.208 <sup>*</sup> (ref 9)	0.208 ± 0.001 (R) 2.88	
303	0.22 (ref 3), 0.19 (ref 7), 0.198* (ref 8), 0.196* (ref 9)	0.201 ± 0.011 (R) 2.78	
313	0.185 <sup>*</sup> (ref 8), 0.182 <sup>*</sup> (ref 9)	0.184 ± 0.002 (R) 2.55	
323	0.178 <sup>*</sup> (ref 8), 0.174 <sup>*</sup> (ref 9)	0.176 ± 0.002 (R) 2.44	
333	0.178 <sup>*</sup> (ref 8), 0.174 <sup>*</sup> (ref 9)	0.176 ± 0.002 (R) 2.44	
343	0.185 <sup>*</sup> (ref 8), 0.179 <sup>*</sup> (ref 9)	0.182 ± 0.003 (R) 2.52	
353	0.199 <sup>*</sup> (ref 8), 0.190 <sup>*</sup> (ref 9)	0.195 ± 0.005 (R) 2.70	
363	0.219 <sup>*</sup> (ref 8), 0.203 (ref 8)	0.211 ± 0.008 (R) 2.92	

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_1)$  have the same status and (relative) percentage uncertainties as the mass % solubilities.

(continued next page)



FIGURE 1. Selected data for the solubility of acetic acid 3-methyl-1-butyl ester (1) in water (2): ref 8 ( $\bullet$ ); ref 9 (O). Solid line is a least square polynomial fitted to the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID 3-METHYL-1-BUTYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid 3-methyl-1-butyl ester (1) are summarized in Table 3 with the following exceptions.

The datum of Bancroft (ref 1) reported in v/v units has been excluded from consideration. The data reported by Othmer et al. (ref 2) and Andreeva et al. (ref 6) are significantly higher than other studies and have been rejected. The data of Iguchi and Fuse (ref 4) and Rao et al. (ref 7) are significantly lower than other studies and are also rejected.

The remaining data, mainly due to Skrzecz (ref 8) and Stephenson and Stuart (ref 9), are in general in good agreement although they differ significantly at T > 343 K. Selected data are plotted in Figure 2.

(continued next page)

12		
СОМРО	NENTS:	EVALUATOR:
(1)	Acetic acid 3-methyl-1-butyl ester ( <i>isopentyl acetate</i> ); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [123-92-2] Water; H <sub>2</sub> O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989
CRITI	CAL EVALUATION: (continued)	
TABLE 3: Recommended (R) and Tentative Solubilities of Water (2) in Acetic acid 3-methyl-1-butyl ester (1)		
1/1	Reported values	"Best" values $(+\sigma)^a$
	g(2)/100g sln	$g(2)/100g \ sln \ 10^2 x_2$
273	0.56 (ref 9)	0.56 3.9
283	0.67 <sup>*</sup> (ref 9)	0.67 4.7
293	0.67 <sup>*</sup> (ref 8), 0.78 <sup>*</sup> (ref 9	0.73 ± 0.06 5.1
298	0.82 <sup>*</sup> (ref 8), 0.82 <sup>*</sup> (ref 9	0.82 (R) 5.6
303	0.58 <sup>b</sup> (ref 3), 0.545 <sup>b</sup> (ref 0.83 <sup>*</sup> (ref 8), 0.87 <sup>*</sup> (ref 9	5) 0.85 ± 0.02 (R) 5.8
313	0.85 <sup>*</sup> (ref 8), 0.96 <sup>*</sup> (ref 9	0.90 ± 0.06 (R) 6.2

 $^a$  Obtained by averaging where appropriate;  $\sigma_{
m n}$  has no statistical significance. Mole fraction solubilities  $(x_2)$  have the same status and (relative) percentage uncertainties as the mass % solubilities.

 $1.11^*$  (ref 8),  $1.13^*$  (ref 9)  $1.12 \pm 0.01$  (R)

 $1.32^*$  (ref 8),  $1.21^*$  (ref 9)  $1.26 \pm 0.06$  (R)

 $1.62^*$  (ref 8),  $1.28^*$  (ref 9)  $1.5 \pm 0.2$ 

 $1.00 \pm 0.05 (R)$ 

 $1.7 \pm 0.4$ 

<sup>b</sup> Not included in calculation of "Best" value.

0.96<sup>\*</sup> (ref 8), 1.05<sup>\*</sup> (ref 9)

2.03<sup>\*</sup> (ref 8), 1.33<sup>\*</sup> (ref 9)

(continued next page)

6.8

7.6

8.5

10

17

323

333

343

353



COMPO	DNENTS:	EVALUATOR:
(1) (2)	Acetic acid 3-methyl-1-butyl ester ( <i>isopentyl acetate</i> ); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [123-92-2] Water; H <sub>2</sub> O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989
CRITI	CAL EVALUATION: (continued)	
8.	Skrzecz, A. Pol. J. Chem. <u>1981</u> , Thesis, I. Ch. F. PAN, Warszawa,	55, 1177-80; see also Skrzecz, A. <u>1979</u> .
9.	Stephenson, R.; Stuart, J. J. C	Chem. Eng. Data <u>1986</u> , 31, 56-70.
ACKNO	DWLEDGEMENT	
	The Evaluator thanks Dr. Brian Cl	lare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid 3-methyl-1-butyl	Bancroft, W.D.	
ester (isopentyl acetate);	Phys. Rev. <u>1895</u> , 3, 114-36.	
(2) Note: $(23-32-2)$		
(2) water; $H_20$ ; [7/32-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid 3-methyl-1-butyl ester in water at 20°C was reported to be 0.02 mL(1)/10mL(2).		
The solubility of water in acetic act reported to be 0.12 mL(2)/10mL(1).	id 3-methyl-1-butyl ester at 20°C was	
AUVILTADV	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. 10 mL of solvent in a test tube	<ul> <li>(1) Laboratory source; dried over CaCl<sub>2</sub>, distilled.</li> </ul>	
was titrated with the second component until the solution	(2) Not specified.	
became Cloudy.		
	ESTIMATED ERROR:	
	Soly. ±0.01 mL.	
	REFERENCES:	

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r		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid 3-methyl-1-butyl     ester (isopentyl acetate);     Que o 1122 22 22</pre>	Othmer, D.F.; White, R.E.; Trueger, E.	
$C_7 H_{14} O_2; [123 - 92 - 2]$	іпа. <i>Eng. Cnem.</i> <u>1941</u> , 33, 1240-8, 1513.	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 297	Z. Maczynska	
EXPERIMENTAL VALUES: The solubility of acetic acid 3-methyl-1-butyl ester in water at 23.5°C was reported to be 0.16 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calculated by the compiler is 2.2 x 10 <sup>-4</sup> . The solubility of water in acetic acid 3-methyl-1-butyl ester at 23.5°C was reported to be 2.8 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calculated by the compiler is 0.172.		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Nothing was specified in the paper.	(1) Not specified.	
	(2) Not specified	
	(2) NOT SPECIFIED.	
	ESTIMATED ERROR:	
	Temp. ±0.5 <sup>0</sup> C (mean of reported	
	<pre>range), Soly. about ±0.04 g(1)/100g sln and ±2.1 g(2)/100g sln (compiler).</pre>	
	REFERENCES:	

1		
ORIGINAL MEASUREMENTS: Narasimhan, K.S.; Reddy, C.C.; Chari, K.S. J. Chem. Eng. Data <u>1962</u> , 7, 457-60.		
PREPARED BY:		
A. Skrzecz		
EXPERIMENTAL VALUES: The solubility of acetic acid 3-methyl-1-butyl ester in water at $30^{\circ}$ C was reported to be 0.22 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calculated by the compiler is $3.1 \times 10^{-4}$ . The solubility of water in acetic acid 3-methyl-1-butyl ester at $30^{\circ}$ C was reported to be 0.58 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calculated by the compiler is 0.040.		
INFORMATION		

**REFERENCES:** 

dexes of both layers were measured

and the corresponding compositions were obtained graphically from a previously drawn plot relating the refractive index and composition.

The data were reported together with the ternary system acetic acid 3-methyl-1-butyl ester-water-

phenol.

 Narasimhan, K.S.; Reddy, C.C.; Chari, K.S. J. Chem. Eng. Data <u>1962</u>, 7, 340. ;

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid 3-methyl-1-butyl	Iguchi, A.; Fuse, K.	
ester (isopentyl acetate);	Kagaku Kogaku <u>1971</u> , 35(9), 1035-7.	
$C_7 R_{14} O_2$ ; $[123 - 92 - 2]$		
(2) water; $H_20$ ; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid 3-methyl-1-butyl ester in water at 25°C was reported to be 0.43 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calculated by the compiler is 6.0 x 10 <sup>-4</sup> . The solubility of water in acetic acid 3-methyl-1-butyl ester at 25°C was reported to be 0.32 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calculated by the compiler is 0.0227.		
λιιντι τλου τησορηλητοή		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. The samples were titrated with the second component to obtain turbi- dity. The method and data were reported together with the ternary system acetic acid 3-methyl-1-butyl ester-water-acetic acid. No further	(1) Source not specified, commer- cial grade of high purity, used as received.	
	(2) Not specified.	
details were reported in the paper.	FOUL FDDOD.	
	Town to 190	
	Temp. $\pm 0.1^{-C}$ . Soly. about $\pm 0.2$ g(1)/100g sln and $\pm 0.4$ g(2)/100g sln (compiler).	
	REFERENCES:	

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1)	Acetic acid 3-methyl-1-butyl ester ( <i>isopentyl acetate</i> ); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [123-92-2]	Ramanarao, M.V.; Husain, A.; Chari, K.S. Indian J. Technol. <u>1964</u> , 2, 252-4.			
(2)	Water; H <sub>2</sub> O; [7732-18-5]				
VARIABLES:		PREPARED BY:			
T/K = 303		A. Skrzecz			

#### EXPERIMENTAL VALUES:

The solubility of acetic acid 3-methyl-1-butyl ester in water at  $30^{\circ}$ C was reported to be 0.2500 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 3.467 x  $10^{-4}$ .

The solubility of water in acetic acid 3-methyl-1-butyl ester at  $30^{\circ}$ C was reported to be 0.5445 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.03806.

AUXTLARY INFOR	MATTON

## METHOD/APPARATUS/PROCEDURE:

The turbidity end point method described by Narasimhan, Reddy and Chari (ref 1) was used. Only the method for the ternary system was described. A known weight of mixture was placed into a 100 mL stoppered conical flask and kept in a thermostat for 1/2 h. which was found to be sufficient for equilibrium. Then, the selected Component was added dropwise until a permanent turbidity appeared in the solution. SOURCE AND PURITY OF MATERIALS:

- (1) Source not specified; twice distilled; b.p. 142.1°C.
- (2) Distilled.

ESTIMATED ERROR:

Temp.  $\pm 0.1^{\circ}C$  (authors). Soly. about  $\pm 0.05$  g(1)/100g sln and  $\pm 0.2$  g(2)/100g sln (compiler).

**REFERENCES:** 

 Narasimhan, K.S.; Reddy, C.C.; Chari, K.S. J. Chem. Eng. Data 1962, 7, 340.

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COMPONENTS:	ORIGINAL MEASUREMENTS:					
(1) Acetic acid 3-methyl-1-butyl ester (isopentyl acetate);	Andreeva, N.G.; Komarova, L.F.; Garber, Yu.N.					
C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [123-92-2]	Zh. Prikl. Khim. <u>1978</u> , 51, 2031-6.					
(2) Water; H <sub>2</sub> O; [7732-18-5]						
VARIABLES:	PREPARED BY:					
T/K = 367	A. Skrzecz					
EXPERIMENTAL VALUES: The solubility of acetic acid 3-methyl-1-butyl ester in water at $94.0^{\circ}C^{a}$ was reported to be $x_{1} = 0.011$ . The corresponding mass per cent value calculated by the compiler is 7.4 g(1)/100g sln. The solubility of water in acetic acid 3-methyl-1-butyl ester at $94.0^{\circ}C^{a}$ was reported to be $x_{2} = 0.179$ . The corresponding mass per cent value calculated by the compiler is 2.93 g(2)/100g sln. <sup>a</sup> Boiling temperature at atmospheric pressure.						
AUXILIARY	INFORMATION					
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:					
The titration method of Mozzhukhin,	(1) Not specified.					
Tyurikov and Mitropolskaya (ref 1) was used. The data were reported	(2) Not specified.					
together with the ternary system acetic acid 3-methyl-1-butyl ester-						
water-acetic acid butyl ester (isopentyl acetate-water-butyl						
acetate). No further details were reported in the paper.						
	ESTIMATED ERROR:					
	Soly. about ±7.2 g(1)/100g sln and ±0.8 g(2)/100g sln (compiler).					
	REFERENCES:					
	<ol> <li>Mozzhukhin, A.S.; Tyurikov, I.D.; Mitropolskaya, V.A. in Fiz. Khim. Osn. Rektifikatsii, Moskva, <u>1970</u>.</li> </ol>					

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ORIGINAL MEASUREMENTS: Rao, D.S.; Rao, K.V.; Prasad, A.R.; Chiranjivi, C. J. Chem. Eng. Data <u>1979</u> , 24, 241-4.
PREPARED BY:
hyl-1-butyl ester in water at $30^{\circ}$ C was the corresponding mole fraction, $x_1$ , 2.6 x $10^{-4}$ . Bid 3-methyl-1-butyl ester at $30^{\circ}$ C was the corresponding mole fraction, $x_2$ , 0.011.
INFORMATION
<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, reagent grade; used as received. (2) Distilled; free from CO<sub>2</sub>.  ESTIMATED ERROR: Temp. ±0.1°C (authors). Soly. about ±0.01 g(1)/100g sln and ±0.6 g(2)/100g sln (compiler). REFERENCES:</pre>

2					
COMPONENTS:	;		ORIGINAL MEASUREMENTS:		
(1) Aceti	ic acid 3-meth	vl-1-butvl	Skrzecz, A.		
ester (isopentyl acetate);			Del 7 Cham 1001 55 1177 00		
C <sub>7</sub> H <sub>14</sub>	02; [123-92-2]		<i>POL. J. CNEM.</i> <u>1981</u> , 55, 1177-80.		
(2) Water	- H.O: [7732-	18-51	Skrzecz, A.		
(2) hater	.,		Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u> .		
VARIABLES:			PREPARED BY:		
T/K = 288	- 359		A. Skrzecz		
EXPERIMENTA	AL VALUES:	agetic agid (	l	or and water	
T/K		x1	g(1)/100	g sln	
(	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase	
288.4 <sup>a</sup>		0,9562		99.370	
296.9	0.00029	-	0.209	_	
306.3	-	0.9470	-	99.231	
310.1	0.00026	-	0.188	-	
320.7	0.00025	-	0.180	-	
325.9	-	0.9304	***	98.975	
339.3	0.00025		0.180	-	
344.4	-	0.9114	-	98.673	
<sup>a</sup> Byt	he Karl Fisch	er method.	(continued next page)		
		AUXILIARY	INFORMATION		
		DF.			
			booken and fokill of mainkined.		
The synthe and the ar used. An a of fixed c in a glass thermostat distilled	etic method of halytical meth mpoule with t concentration s tube connect filled compl water. During	Alexejew od were he solution was placed ed with a etely with the meas-	<ul> <li>(1) Prolabo-Rhone Poulene, pure grade; distilled; purity 99.97% by glc, 0.08 wt% water by the Karl Fischer method.</li> <li>(2) Distilled.</li> </ul>		
urements t	he temperatur	e of the			
the appear	ance and disa	ppearance of	ESTIMATED ERROR:		
turbidity observed v cal method the satura determined	within the am visually. For I, The amount Ited organic p I using a Karl	poule was the analyti- of water in hase was Fischer	Temp. ±(0.2-0.6) <sup>o</sup> C. Soly. see above.		
titration procedure. The amount of water in the pure ester was taken into account.			REFERENCES:	- <u></u>	
COMPONENTS:	ORIGINAL MEASUREMENTS:				
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<ul> <li>(1) Acetic acid 3-methyl-1-butyl ester (<i>isopentyl acetate</i>); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>; [123-92-2]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	Skrzecz, A. <i>Pol. J. Chem.</i> <u>1981</u> , 55, 1177-80. Skrzecz, A. <i>Thesis</i> , Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u> .				
EXPERIMENTAL VALUES: (continued) Mutual solubility of acetic acid 3 T/K X <sub>1</sub> (2)-rich phase (1)-rich phas	-methyl-1-butyl ester and water g(1)/100g sln e (2)-rich phase (1)-rich phase				

345.5	0.00026		0.188	-
358.6	0.00029	-	0.209	-
358.8	-	0.8804	-	98.155

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Author's smoothing equations:
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\begin{aligned} x_1 &= 3.680 \times 10^{-4} - 4.37 \times 10^{-6} (T/K - 273.15) + 3.98 \times 10^{-8} (T/K - 273.15)^2 \\ &\text{st.dev.} = 1.82 \times 10^{-6} (2) - \text{rich phase} \\ x_2 &= 0.038754 + 2.150 \times 10^{-4} (T/K - 273.15) + 6.82 \times 10^{-6} (T/K - 273.15)^2 \end{aligned}
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st. dev. =  $6.68 \times 10^{-4}$  (1)-rich phase

(1) Acetic acid 3-methyl-1-butyl ester (isopentyl acetato); CyH <sub>14</sub> O <sub>2</sub> ; (123-92-2)       Stephenson, R.; Stuart, J.         (2) Water; H <sub>2</sub> O; (7732-18-5)       J. Chem. Eng. Data 1996, 31, 56-70.         (2) Water; H <sub>2</sub> O; (7732-18-5)       PREPARED BY:         Z. Maczynska       Z. Maczynska         Mutual solubility of acetic acid 3-methyl-1-butyl ester and water       Image: Component (2)-rich phase (1)-rich phase         (2)-rich phase (1)-rich phase       (2)-rich phase (1)-rich phase         (3) 0.30       0.206       99.20       0.000240       0.9475         30.3       0.208       99.20       0.000250       0.9416         50.0       0.174       98.89       0.000241       0.9250         60.1       0.152       98.84       0.000220       0.913         70.2       0.205       98.66       0.000284       0.9106          0.000284       0.9106       0.000284       0.9106          0.000284       0.9106       0.000284       0.9106          0.000284       0.91	COMPONENT	rs:		ORIGINAL MEASUREM	ENTS:
ester (isopentyl acetate); C,H <sub>14</sub> O <sub>2</sub> ; [123-92-2]       J. Chem. Eng. Data 1986, 31, 56-70.         (2) Water; H <sub>2</sub> O; (7732-18-5)       PREPARED BY:         //RIABLES:       PREPARED BY:         Z/K = 273 - 364       Z. Maczynska         XXPERIMENTAL VALUES:       Mutual solubility of acetic acid 3-methyl-1-butyl ester and water         t/ <sup>0</sup> C       g(1)/100g sln       x1 (compiler)         (2)-rich phase (1)-rich phase       (2)-rich phase (1)-rich phase         0       0.340       99.44       0.000472       0.9609         9.1       0.265       99.33       0.000286       0.9473         30.3       0.208       99.20       0.000286       0.9416         50.0       0.174       98.89       0.000210       0.9218         50.1       0.152       98.76       0.000281       0.9168         80.3       0.182       98.80       0.000222       0.9133         90.7       0.205       98.66       0.000284       0.9106         AUXILIARY INFORMATION         EFTIMOD/APPARATUS/PROCEDURE:         The analytical method was used.         Component (1) was equilibrated       (2) Not specified.         with component (2) ata givon       as received.	(1) Ace	etic acid 3-methy	vl-1-butyl	Stephenson, R.; S	Stuart, J.
(2) Water; H <sub>2</sub> O; [7732-18-5]         /ARIABLES:         T/K = 273 - 364         EXPERIMENTAL VALUES:         Mutual solubility of acetic acid 3-methyl-1-butyl ester and water         t/°C       g(1)/100g sln         x1 (compiler)         (2)-rich phase (1)-rich phase         0       0.340         9.1       0.265         9.1       0.265         9.1       0.268         9.7       0.184         9.7       0.184         9.7       0.184         9.7       0.182         9.8.8       0.000281         0.00225       0.918         70.2       0.203         98.76       0.000281         0.152       98.86         0.00028       0.9106         std. dev.       0.002         AUXILIARY INFORMATION    AUXILIARY INFORMATION          ETHOD/APPARATUS/PROCEDURE:    The analytical method was used. Companic 1(1) was equilibrated with component (2) at a given temperature in a thermostat. Each Harmotical sample; purity 99%; u as recieda. (2) Not specified. (2) Not	est C <sub>7</sub> H	ter ( <i>isopentyl ac</i> 1 <sub>14</sub> 0 <sub>2</sub> ; [123-92-2]	cetate);	J. Chem. Eng. Dat 56-70.	ta <u>1986</u> , 31,
DARIABLES:PREPARED BY: $T/K = 273 - 364$ Z. MaczynskaZXPERIMENTAL VALUES:Mutual solubility of acetic acid 3-methyl-1-butyl ester and water $t/^{\circ}C$ $g(1)/100g sln$ $(2)$ -rich phase (1)-rich phase $x_1$ (compiler) $(2)$ -rich phase (1)-rich phase $(2)$ -rich phase (1)-rich phase $0$ $0.340$ $99.44$ $0.000472$ $0.00255$ $99.33$ $0.000367$ $0.9535$ $19.4$ $0.212$ $99.20$ $0.000288$ $99.7$ $0.184$ $99.15$ $0.000288$ $99.7$ $0.184$ $99.15$ $0.000288$ $50.0$ $0.174$ $98.89$ $0.000241$ $50.0$ $0.174$ $98.89$ $0.000281$ $70.2$ $0.203$ $98.76$ $0.000281$ $70.2$ $0.203$ $98.76$ $0.000221$ $90.7$ $0.205$ $98.66$ $0.000284$ $0.9105$ $0.002$ $0.01$ AUXILIARY INFORMATIONETHOD/APPARATUS/FROCEDURE:The analytical method vas used.Component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed anount of acetonitrile organic layer sample and measuring T390 A recorder-integrator).SURCE AND PURITY OF MATERIALS: (2) Not specified.(2) Not specified (determine (2) in the was used to determine (2) in the <b< td=""><td>(2) Wat</td><td>ter; H<sub>2</sub>O; [7732-1</td><td>.8-5]</td><td></td><td></td></b<>	(2) Wat	ter; H <sub>2</sub> O; [7732-1	.8-5]		
$T/K = 273 - 364$ 2. Maczynska         EXPERIMENTAL VALUES:       Mutual solubility of acetic acid 3-methyl-1-butyl ester and water $t/^{\circ}C$ g(1)/100g sln $x_1$ (compiler)         (2)-rich phase (1)-rich phase       (2)-rich phase (1)-rich phase       (2)-rich phase (1)-rich phase         0       0.340       99.44       0.000472       0.9609         9.1       0.265       99.33       0.000367       0.9535         19.4       0.212       99.24       0.000228       0.9445         30.3       0.208       99.20       0.000288       0.9445         50.0       0.174       98.89       0.000210       0.9218         70.2       0.203       98.76       0.000281       0.9108         70.2       0.203       98.76       0.000281       0.9106         80.3       0.182       98.80       0.000281       0.9106         AUXILIARY INFORMATION         AUXILIARY INFORMATION         ETHOD/APPARATUS/FROCEDURE:         The analytical method vas used.         Component (2) was equilibrated or adding a weighed anount of acetonitrile or adding a weighed anount of acetonitrile conductivity gate determined by adding a weighed anount of acetonitrile conductivity gate coreduce-integrator).	VARIABLES	5:		PREPARED BY:	
XPERIMENTAL VALUES:           Mutual solubility of acetic acid 3-methyl-1-butyl ester and water $t/^{OC}$ g(1)/100g sln $x_1$ (compiler)           (2)-rich phase (1)-rich phase         (2)-rich phase (1)-rich phase         (2)-rich phase (1)-rich phase           0         0.340         99.44         0.000472         0.9609           9.1         0.265         99.33         0.000367         0.9535           19.4         0.212         99.24         0.000294         0.9475           30.3         0.208         99.20         0.000286         0.9449           39.7         0.184         99.15         0.000281         0.9250           60.1         0.152         98.84         0.000210         0.92168           80.3         0.182         98.80         0.000281         0.9168           AUXILIARY INFORMATION           AUXILIARY INFORMATION           AUXILIARY INFORMATION           AUXILIARY INFORMATION           AUXILIARY INFORMATION           AUXILIARY INFORMATION           Component (2) at a given tamper, tampro, tamper, tamper, tamper, tamper, tamper, tamper, tamper,	T/K = 27	73 - 364		Z. Maczynska	
Mutual solubility of acetic acid 3-methyl-1-butyl ester and water $t/^{OC}$ g(1)/100g sln $x_1$ (compiler)           (2)-rich phase (1)-rich phase         (2)-rich phase (1)-rich phase           0         0.340         99.44         0.000472         0.9609           9.1         0.265         99.33         0.000367         0.9535           19.4         0.212         99.24         0.000294         0.9445           30.3         0.208         99.20         0.000288         0.9449           39.7         0.184         99.15         0.000255         0.9416           50.0         0.174         98.89         0.000210         0.9218           70.2         0.203         98.76         0.000281         0.9168           80.3         0.182         98.80         0.000284         0.9106           AUXILIARY INFORMATION    ETHOD/APPARATUS/PROCEDURE:  The analytical method was used. Component (1) was eguilibrated with component (2) at a given temperature in a thermostat. Each temperature in a thermostat. Each temperature in a thermostat. Each temperature in a thermostat. Particle (Or sometimes propanol) to the organic layer sample and measuring by a Gou-Mac thermal conductivity go the (1)/acetonitrile peak ratio (Othomosorb 101 packing and HP 390 A recorder-integrator). A similar procedure but a higher boiling material (a.9. 1-hexanol) was used to determine (	EXPERIMEN	NTAL VALUES:			
$\frac{t/^{9}C}{(2)-rich phase (1)-rich phase} (2)-rich phase (1)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (1)-ric$	Mutua	al solubility of	acetic acid 3.	-methyl-1-butyl es	ter and water
(2)-rich phase (1)-rich phase00.34099.440.0004720.96099.10.26599.330.0003670.953519.40.21299.240.000280.944530.30.20899.200.0002880.944939.70.18499.150.0002550.941650.00.17498.890.0002100.921860.10.15298.840.0002100.921870.20.20398.760.0002810.916880.30.18298.800.0002250.919390.70.20598.660.0002840.9106std. dev. 0.0020.01LETHOD/APPARATUS/PROCEDURE:The analytical method was used. Component (1) was equilibrated wighed amount of acetonitrile (Or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity of ch (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP aya used to determine (2) in the water layer.SOURCE AND FURITY OF MATERIALS: SOURCE AND FURITY OF MATERIALS: SOURCE AND FURITY OF MATERIALS: Corracy of method 0.1 wt% or for solubility, see above.REPERENCES:	t/°C	g(1)/10	0g sln	$x_1$ (comp	oiler)
0         0.340         99.44         0.000472         0.9609           9.1         0.265         99.33         0.000367         0.9535           19.4         0.212         99.24         0.000294         0.9475           30.3         0.208         99.20         0.000288         0.9449           39.7         0.184         99.15         0.000255         0.9416           50.0         0.174         98.89         0.000210         0.9218           70.2         0.203         98.76         0.000281         0.9168           80.3         0.182         98.80         0.000252         0.9193           90.7         0.205         98.66         0.000284         0.9106           ETHOD/APPARATUS/PROCEDURE:           The analytical method was used.         Component (1) was equilibrated         (1) Source not specified, comm cial sample; purity 99%; u as received.           tamperature in a thermostat. Each layer was sampled with a syringe; to a gov-Mac thermal conductivity go the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP atoral)         SOURCE AND PURITY OF MATERIALS:           3300 A recorder-integrator).         A similar procedure but a higher boiling material (e.g. 1-hexanol)         Accuracy of method 0.1 wt% or for solubility, see above.           Notility see todetermine (2)		(2)-rich phase	(1)-rich phase	e (2)-rich phase	(1)-rich phase
9.1       0.265       99.33       0.000367       0.9535         19.4       0.212       99.24       0.000294       0.9475         30.3       0.208       99.20       0.000288       0.9449         39.7       0.184       99.15       0.000255       0.9416         50.0       0.174       98.89       0.000210       0.9218         70.2       0.203       98.76       0.000281       0.9168         80.3       0.182       98.80       0.000252       0.9193         90.7       0.205       98.66       0.000284       0.9106         AUXILIARY INFORMATION    ETHOD/APPARATUS/PROCEDURE:          The analytical method was used.       Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (0r sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity go the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3300 A recorder-integrator).       Source AND PURITY OF MATERIALS:         As similar procedure but a higher bolling material (e.g. 1-hexanol)       References:         Nature layer.       References:	0	0.340	99.44	0.000472	0.9609
19.4       0.212       99.24       0.000294       0.9475         30.3       0.208       99.20       0.000288       0.9449         39.7       0.184       99.15       0.000255       0.9416         50.0       0.174       98.89       0.000241       0.9256         60.1       0.152       98.84       0.000210       0.9218         70.2       0.203       98.76       0.000281       0.9168         80.3       0.182       98.80       0.000252       0.9193         90.7       0.205       98.66       0.000284       0.9106         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         The analytical method was used.         Component (1) was equilibrated       SOURCE AND PURITY OF MATERIALS:         (1) was determined by adding a       weighed amount of acetonitrile       SOURCE AND PURITY OF MATERIALS:         (2) Not specified.       (2) Not specified.       (2) Not specified.         (2) Not specified.       (2) Not specified.       (2) Not specified.         STIMATED ERROR:         Accuracy of method 0.1 wt% or for solubility, see above.         Mayer was used to determine (2) in the water layer.       REFERENCES:	9.1	0.265	99.33	0.000367	0.9535
30.30.20899.200.0002880.944939.70.18499.150.0002550.941650.00.17498.890.0002100.921870.20.20398.760.0002810.916880.30.18298.800.0002520.919390.70.20598.660.0002840.9106AUXILIARY INFORMATIONEETHOD/APPARATUS/PROCEDURE:The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.SURCE AND PURITY OF MATERIALS: SURCE AND PURITY OF MATERIALS: SURCE AND PURITY OF MATERIALS: (2) Not specified.ESTIMATED ERROR: Accuracy of method 0.1 wt% or for solubility, see above.REFERENCES:	19.4	0.212	99.24	0.000294	0.9475
39.70.18499.150.0002550.941650.00.17498.890.0002410.925060.10.15298.840.0002100.921870.20.20398.760.0002810.916880.30.18298.800.0002520.919390.70.20598.660.0002840.9166std. dev. 0.0020.01Ketthod/APPARATUS/PROCEDURE:The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sample and with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb Ol packing and at HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.SURCE AND PURITY OF material with or for solubility, see above.REFERENCES:	30.3	0.208	99.20	0.000288	0.9449
50.00.17498.890.0002410.925060.10.15298.840.0002100.921870.20.20398.760.0002810.916880.30.18298.800.0002520.919390.70.20598.660.0002840.9106AUXILIARY INFORMATIONETHOD/APPARATUS/PROCEDURE:The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gy a the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.Source size above.ESTIMATED ERROR: Accuracy of method 0.1 wt% or for solubility, see above.REFERENCES:	39.7	0.184	99.15	0.000255	0.9416
60.10.15298.840.0002100.921870.20.20398.760.0002810.916880.30.18298.800.0002520.919390.70.20598.660.0002840.9106AUXILIARY INFORMATIONKETHOD/APPARATUS/PROCEDURE:The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gy a the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.Source sizeESTIMATED ERROR: Accuracy of method 0.1 wt% or for solubility, see above.REFERENCES:	50.0	0.174	98.89	0.000241	0.9250
70.2       0.203       98.76       0.000281       0.9168         80.3       0.182       98.80       0.000252       0.9193         90.7       0.205       98.66       0.000284       0.9106         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         The analytical method was used.         Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe;       SOURCE AND PURITY OF MATERIALS:         (1) Was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).       Source and source above.         A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.       REFERENCES:         REFERENCES:	60.1	0.152	98.84	0.000210	0.9218
80.3       0.182       98.80       0.000252       0.9193         90.7       0.205       98.66       0.000284       0.9106         Std. dev. 0.002       0.01         AUXILIARY INFORMATION         AUXILIARY INFORMATION         ETHOD/APPARATUS/PROCEDURE:         The analytical method was used.         Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe;         (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.       Source and period 0.1 wt% or for solubility, see above.         REFERENCES:	70.2	0.203	98.76	0.000281	0.9168
90.7       0.205       98.66       0.000284       0.9106         std. dev. 0.002       0.01         AUXILIARY INFORMATION         AUXILIARY INFORMATION         AUXILIARY INFORMATION         Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a Hp 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.       SOURCE AND PURITY OF MATERIALS: (1) Source not specified, comm cial sample; purity 99%; u as received.         SOURCE AND PURITY OF MATERIALS: (1) Source not specified, comm cial sample; purity 99%; u as received.         (2) Not specified.         ESTIMATED ERROR: Accuracy of method 0.1 wt% or for solubility, see above.         REFERENCES:	80.3	0.182	98.80	0.000252	0.9193
std. dev. 0.002       0.01         AUXILIARY INFORMATION         AUXILIARY INFORMATION         SOURCE AND PURITY OF MATERIALS:         Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.       SOURCE AND PURITY OF MATERIALS:         REFERENCES:	90.7	0.205	98.66	0.000284	0.9106
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Source not specified, comm cial sample; purity 99%; u as received. (2) Not specified. (2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or for solubility, see above. REFERENCES: REFERENCES:	sta. c	lev. 0.002	0.01		
<pre>SOURCE AND PURITY OF MATERIALS: The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.</pre> SOURCE AND PURITY OF MATERIALS: (1) Source not specified, comm cial sample; purity 99%; u as received. (2) Not specified. (2) Not specified. (3) Source and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (2) Not specified. (3) Source and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP soliling material (e.g. 1-hexanol) was used to determine (2) in the water layer. REFERENCES:			AUXILIARY II	NFORMATION	
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. (1) Source not specified, comm cial sample; purity 99%; u as received. (2) Not specified. (2) Not specified. (2) Not specified. (3) Source not specified, comm cial sample; purity 99%; u as received. (2) Not specified. (3) Source not specified, comm cial sample; purity 99%; u as received. (2) Not specified. (2) Not specified. (3) Source not specified, comm cial sample; purity 99%; u as received. (2) Not specified. (3) Source not specified, comm cial sample; purity 99%; u as received. (2) Not specified. (3) Source not specified, comm cial sample; purity 99%; u as received. (2) Not specified. (3) Source not specified. (4) Source not specified, comm cial sample; purity 99%; u as received. (2) Not specified. (3) Source not specified. (4) Source not specified. (5) Source not specified. (2) Not specified. (3) Source not specified. (4) Source not specified. (5) Source not specified. (5) Source not specified. (6) Source not specified. (6) Source not specified. (7) Source not specified. (7) Source not specified. (8) Source not specified. (8) Source not specified. (8) Source not specified. (9) Source not specified. (9) Source not specified. (1) Source not specified. (2) Not specified. (3) Source not specified. (4) Source not specified. (5) Source not specified. (6) Source not specified. (6) Source not specified. (7) Source not specified. (8) Source not specified. (8) Source not specified. (8) Source not specified. (8) Sourc	METHOD/AP	PARATUS/PROCEDUR	E:	SOURCE AND PURITY	OF MATERIALS:
<ul> <li>(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).</li> <li>A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.</li> <li>(2) Not specified.</li> </ul>	The anal Componen with com	ytical method wa ht (1) was equili hponent (2) at a	s used. brated given	(1) Source not sr cial sample; as received.	pecified, commer purity 99%; use
organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. REFERENCES:	(1) was weighed (or some	is sampled with a determined by ad amount of aceton stimes propanol)	syringe; ding a itrile to the	(2) Not specified	ł.
<pre>gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. REFERENCES: REFERENCES:</pre>	organic by a Corr	layer sample and	measuring	ESTIMATED ERROR:	
3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. REFERENCES:	gc the ( (Chromos	1)/acetonitrile orb 101 packing	peak ratio and a HP	Accuracy of metho	od 0.1 wt% or le
was used to determine (2) in the water layer. REFERENCES:	3390 A r A simila boiling	ecorder-integrat r procedure but material (e.g. 1	or). a higher -hexanol)	for solubility, s	ee above.
	was used water la	yer.	, in the	REFERENCES:	

f

COMPO	DNENTS:	EVALUATOR:
(1)	Acetic acid pentyl ester (pentyl acetate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[628-63-7]	Murdoch University, Perth, W.A.,
(2) Water: H_O: [7732-18-5]	Australia	
		January, 1989

CRITICAL EVALUATION:

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

<u>TABLE 1: Quantine Acetic acid pent</u>	tative Sol yl ester	lubility Studies (1) - Water (2) S	of the System
Reference	T/K	Solubility	Method
Hemptinne (ref 1)	298	(1) in (2)	analytical
Park and Hopkins (ref 2)	298	(1) in (2)	unspecified
Doolittle (ref 3)	293	mutual	unspecified
Rao and Rao (ref 4)	303	mutual	titration
Venkataratnam <i>et al</i> . (ref 5)	303	mutual	titration
Rao and Rao (ref 6)	303	mutual	titration
Krupatkin and Shcherbakova (ref 7)	298	mutual	titration
Skrzecz (ref 8)	286-365	mutual	synthetic, Karl Fischer
Richon and Viallard (ref 9)	298	mutual	calorimetric, refractometric
Stephenson and Stuart (ref 10)	273-364	mutual	GLC

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. SOLUBILITY OF ACETIC ACID PENTYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid pentyl ester (1) in water (2) are summarized in Table 2 with the following exclusions. The datum of Park and Hopkins (ref 2) reported in v/v units has been excluded from consideration. The datum of Krupatkin and Shcherbakova (ref 7) and the approximate values of Rao et al. (ref 4-6) appear to be high and have been rejected. Selected data are plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) Acetic acid pentyl ester   (pentyl acetate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;</pre>	G.T. Hefter, School of Mathematical and Physical Sciences,
[628-63-7]	Murdoch University, Perth, W.A.,
(2) Water; H <sub>2</sub> O; [7732-18-5]	Australla January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2:	Recommen	ded (R)	and Ten	<u>tative</u>	Solubil	<u>ities</u>
of A	cetic acid	pentyl	ester (1	) in W	later (2	2

T/K	Solubilities		
	Reported values	"Best" values (± $\sigma$	n) <sup>a</sup>
	g(1)/100g sln	g(1)/100g sln	10 <sup>4</sup> x <sub>1</sub>
273	0.29 (ref 10)	0.29	4.0
283	0.224 <sup>*</sup> (ref 8), 0.25 <sup>*</sup> (ref 10)	0.24 ± 0.01 (R)	3.3
293	0.195 <sup>*</sup> (ref 8), 0.22 <sup>*</sup> (ref 10)	0.21 ± 0.01 (R)	2.9
298	0.162 <sup>*</sup> (ref 1), 0.183 <sup>*</sup> (ref 8), 0.178 <sup>*b</sup> (ref 9), 0.19 <sup>*</sup> (ref 10)	0.178 ± 0.010 (R)	2.46
303	0.172 <sup>*</sup> (ref 8), 0.18 <sup>*</sup> (ref 10)	0.176 ± 0.004 (R)	2.44
313	0.157 <sup>*</sup> (ref 8), 0.15 <sup>*</sup> (ref 10)	0.154 ± 0.004 (R)	2.13
323	0.150 <sup>*</sup> (ref 8), 0.10 (ref 10)	0.13 ± 0.02	1.8
333	0.151 <sup>*</sup> (ref 8), 0.10 <sup>*</sup> (ref 10)	0.13 ± 0.02	1.8
343	0.161 <sup>*</sup> (ref 8), 0.17 <sup>*</sup> (ref 10)	0.166 ± 0.005 (R)	2.30
353	0.181 <sup>*</sup> (ref 8), 0.17 <sup>*</sup> (ref 10)	0.176 ± 0.006 (R)	2.44
363	0.211 <sup>*</sup> (ref 8)	0.21	2.9

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_1)$  have the same status and (relative) percentage uncertainties as the mass % solubilities.

<sup>b</sup> Average of two independent results reported by the original authors.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID PENTYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid pentyl ester (1) are summarized in Table 3 with the following exceptions.

The approximate values of Rao *et al.* (ref 4-6) are widely scattered and do not add any extra information to the more precise studies (ref 8-10) available and so have been rejected. The datum of Krupatkin and Shcherbakova (ref 7) at 298 K is significantly higher than all other studies (ref 8-10) and has also been rejected. Selected data are plotted in Figure 2.

(continued next page)

COMPO	DNENTS:	EVALUATOR:
(1)	Acetic acid pentyl ester (pentyl acetate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[628-63-7]	Murdoch University, Perth, W.A.,
(2) Water: H <sub>2</sub> O: [7732-18-5]	Australia	
(-)		January, 1989

# CRITICAL EVALUATION: (continued)

Although the remaining data (ref 8-10) are in reasonable agreement over a wide temperature range the differences are generally too large to permit many values to be Recommended without further studies.



FIGURE 1. Selected data for the solubility of acetic acid pentyl ester (1) in water (2): ref 8 ( $\bullet$ ); ref 10 (O). Solid line is a least square polynomial fitted to the "Best" values from Table 2.

(continued next page)

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COMPC	DNENTS:	EVALUATOR:
(1)	Acetic acid pentyl ester	G.T. Hefter, School of Mathematical
	(pentyl acetate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	and Physical Sciences,
	[628-63-7]	Murdoch University, Perth, W.A.,
(2) Water: $H_{-}O$ : $[7732-18-5]$		Australia
(2)		January, 1989

CRITICAL EVALUATION: (continued)

# TABLE 3: Recommended (R) and Tentative Solubilities of Water (2) in Acetic acid pentyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm \sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln $10^2 x_2$	
273	0.79 (ref 10)	0.79 5	
283	0.64 <sup>*</sup> (ref 8), 0.81 <sup>*</sup> (ref 10)	0.73 ± 0.09 5.1	
293	0.63 <sup>*</sup> (ref 8), 0.87 <sup>*</sup> (ref 10)	0.75 ± 0.12 5.2	
298	0.65 <sup>*</sup> (ref 8), 0.91 (ref 9), 0.91 <sup>*</sup> (ref 10)	0.82 ± 0.12 5.6	
303	0.67 <sup>*</sup> (ref 8), 0.96 <sup>*</sup> (ref 10)	0.82 ± 0.14 5.6	
313	0.75 <sup>*</sup> (ref 8), 1.06 <sup>*</sup> (ref 10)	0.9 ± 0.2 6	
323	0.88 <sup>*</sup> (ref 8), 1.16 <sup>*</sup> (ref 10)	1.02 ± 0.14 6.9	
333	1.04 <sup>*</sup> (ref 8), 1.26 <sup>*</sup> (ref 10)	1.15 ± 0.11 7.8	
343	1.25 <sup>*</sup> (ref 8), 1.34 <sup>*</sup> (ref 10)	1.30 ± 0.05 (R) 8.7	
353	1.51 <sup>*</sup> (ref 8). 1.44 <sup>*</sup> (ref 10)	1.48 ± 0.04 (R) 9.8	
363	1.80* (ref 8), 1.55* (ref 10)	1.68 ± 0.13 11	

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_2)$  have the same status and (relative) percentage uncertainties as the mass solubilities.

(continued next page)



COMPONENTS:		EVALUATOR:		
(1)	Acetic acid pentyl ester ( <i>pentyl acetate</i> ); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [628-63-7] Water; H <sub>2</sub> O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989		
CRITI	CAL EVALUATION: (continued)			
8.	Skrzecz, A. Pol. J. Chem. <u>1980</u> , Thesis, I. Ch. F. PAN, Warszawa,	54, 1101-4; see also Skrzecz, A. <u>1979</u> .		
9.	Richon, D.; Viallard, A. Fluid	Phase Equil. <u>1985</u> , 21, 279-93.		
10.	Stephenson, R.; Stuart, J. J. C	Chem. Eng. Data <u>1986</u> , 31, 56-70.		
ACKNO	DWLEDGEMENT			
	The Evaluator thanks Dr. Brian Cl	are for the graphics.		

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Acetic acid pentyl ester	Hemptinne, A.		
(pentyl acetate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [628-63-7]	Z. Phys. Chem. <u>1894</u> , 13, 561-9.		
(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 298	A. Skrzecz		
EXPERIMENTAL VALUES: The solubility of acetic acid pentyl to be 1.622 g(1)/L sln.	ester in water at 25°C was reported		
AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCEDURE:	SOURCE AND PURTTY OF MATERIALS.		
The analytical method was used. The mixture of water with excess ester was heated for some time in a water bath and the ester phase was filtered. A sample of known volume was then transferred to a smaller flask, heated with the known amount of baryta until complete saponifi- cation was obtained and then ti- trated. No further details were	<pre>(1) Not specified. (2) Not specified. ESTIMATED ERROR:</pre>		
reported in the paper.	Not specified. REFERENCES:		

32		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid pentyl ester	Park, J.G.; Hopkins, M.B.	
(pentyl acetate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	Ind. Eng. Chem. <u>1930</u> , 22, 826-30.	
[628-63-7]		
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	A. Skrzecz	
The solubility of acetic acid penty to be 0.2 mL(1)/100mL(2).	l ester in water at 25°C was reported	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Source not specified, commer- cial samples; used as received.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid pentyl ester (pentyl acetate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>; [628-63-7]</pre>	Doolittle, A.K. Ind. End. Chem. <u>1935</u> , 27, 1169-79.	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES: T/K = 293	PREPARED BY: A. Skrzecz	

# EXPERIMENTAL VALUES:

The solubility of acetic acid pentyl ester in water at 20°C was reported to be 0.17 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 2.4 x  $10^{-4}$ .

The solubility of water in acetic acid pentyl ester at 20°C was reported to be 1.15 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.0776.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The method was not specified.	<ul> <li>(1) Source not specified, commercial product; purity 84%, mixed isomers; b.p. range 127-155°C, d<sub>4</sub><sup>20</sup> 0.862.</li> <li>(2) Not specified.</li> </ul>		
	ESTIMATED ERROR:		
	Soly. about ±0.03 g(1)/100g sln and ±0.5 g(2)/100g sln (compiler).		
	REFERENCES:		

COMPONENTES	ODICINAL MEASUDEMENDS.		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Acetic acid pentyl ester	Rao, J.R.; Rao, C.V.		
$(pentyl acetate); C_7 H_{14} O_2;$	J. Appl. Chem. <u>1957</u> , 7, 435-9.		
(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 303	A. Skrzecz		
EXPERIMENTAL VALUES:			
The solubility of acetic acid pentyl	ester in water at 30°C was reported		
lated by the compiler is 6 x $10^{-4}$ .	unding mole fraction, $x_1$ , value calcu-		
Inter by the compiler is o'x io .			
The solubility of water in acetic aci	id pentyl ester at 30°C was reported		
to be 1.7 g(2)/100g sln. The correspo	onding mole fraction, $x_2$ , value calcu-		
lated by the compiler is 0.111.			
AUXILIARY :	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The titration method was used.	(1) May and Baker, reagent grade;		
The data and method were reported together with the ternary system	95% was distilled between 120 and $150^{\circ}$ C. $d^{30}$ 0.8630		
acetic acid pentyl ester-water-	$n_{\rm D}^{30}$ 1.3937.		
	(2) Distilled; free from CO <sub>2</sub> .		
	ESTIMATED ERROR:		
	Temp. $\pm 0.02^{\circ}C$ (authors).		
	Soly. about $\pm 0.2$ g(1)/100g sln and		
	(compiler).		
	REFERENCES:		

	35	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ol> <li>Acetic acid pentyl ester</li> <li>(pentyl acetate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;</li> </ol>	Venkataratnam, A.; Rao, J.R.; Rao, C.V.	
[628-63-7] (2) Water; H <sub>2</sub> O; [7732-18-5]	chem. Eng. Sci. <u>1957</u> , 7, 102-10.	
VARIABLES:	PREPARED BY:	
T/K = 303	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid pentyl ester in water at $30^{\circ}C$ was reported to be 0.2 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calcu- lated by the compiler is 3 x $10^{-4}$ . The solubility of water in acetic acid pentyl ester at $30^{\circ}C$ was reported to be 0.4 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calcu- lated by the compiler is 0.03.		

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: The titration method described by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system acetic acid pentyl ester- water-2-propanone (pentyl acetate- water-acetone).	<pre>SOURCE AND PURITY OF MATERIALS: (1) May and Baker, analytical grade; used as received; 95% distilled between 120 and 150°C. d<sup>30</sup> 0.8630, n<sup>30</sup> 1.3937. (2) Distilled; free of CO<sub>2</sub>. ESTIMATED ERROR: Soly. about ±0.03 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler). REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. 1941, 33, 1240.</pre>			

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	1		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Acetic acid pentyl ester	Rao, J.R.; Rao, C.V.		
(pentyl acetate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	J. Appl. Chem. <u>1959</u> , 9, 69-73.		
(2) Water; $H_20$ ; $[7732-18-5]$			
VARIABLES:	PREPARED BY:		
T/K = 303	A. Skrzecz		
EXPERIMENTAL VALUES: The solubility of acetic acid pentyl ester in water at 30°C was reported to be 0.4 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calcu- lated by the compiler is 6 x 10 <sup>-4</sup> . The solubility of water in acetic acid pentyl ester at 30°C was reported to be 0.9 g(2)/100g sln and 99.2 g(1)/100g sln <sup>a</sup> . The corresponding mole			
fraction, $x_2$ , value calculated by the	compiler is 0.06.		
<sup>a</sup> The sum of mass percent values is	not equal 100%.		
AUXILIARY	INFORMATION		
	CONDOL AND DUDTRY OF NAMEDIAL C.		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Presumably the titration method described by Rao and Rao (ref 1) was used. The data were reported together with the ternary system	(1) May and Barker, analytical grade; 95% had distilled between 120 and 150°C, $d^{30}$ 0.8630, $n_{\rm D}^{30}$ 1.3937.		
acetic acid pentyl ester-water- 1-propanol.	(2) Distilled.		
	ESTIMATED ERROR:		
	Soly. about ±0.2 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).		
	REFERENCES:		
	1. Rao, J.R.; Rao, C.V. J. Appl. Chem. <u>1957</u> , 7, 435.		

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) Acetic acid pentyl ester  (pentyl acetate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;  [628-63-7]</pre>	Krupatkin, I.L.; Shcherbakova, T.A. Zh. Prikl. Khim. <u>1971</u> , 44, 307-11.		
(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES: T/K = 298	PREPARED BY: A. Skrzecz		
The solubility of acetic acid pentyl to be 0.22 g(1)/100g sln. The corresp culated by the compiler is 3.05 x 10 <sup>-</sup> The solubility of water in acetic aci to be 1.20 g(2)/100g sln. The corresp culated by the compiler is 0.0807.	ester in water at 25°C was reported conding mole fraction, $x_1$ , value cal- <sup>4</sup> . id pentyl ester at 25°C was reported conding mole fraction, $x_2$ , value cal-		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		

- The titration method was used. The amount of water in pure ester was taken into account. The data were reported together with the ternary system acetic acid pentyl ester-water-phosphoric acid.
  - (1) Source not specified, analytical grade; b.p. range 147-150°C.
  - (2) Twice distilled.

ESTIMATED ERROR:

Temp.  $\pm 0.1^{\circ}C$  (authors). Soly. about  $\pm 0.03$  g(1)/100g sln and  $\pm 0.5$  g(2)/100g sln (compiler).

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COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Acetic acid pentyl ester			Skrzecz A		
(1) Acetic acid pentyl ester (pentyl acetate): C-H, 40;					
[628-63-7]			Pol. J. Chem. <u>1980</u> , 54, 1101-4.		
(2) Watow, $H_{0}$ , $[7732-18-5]$			Skrzecz, A.		
(2) 11400	2, 120, [,,52	10 0]	Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u> .		
VARIABLES:			PREPARED BY:		
T/K = 286	- 365		A. Skrzecz		
EXPERIMENTAL VALUES: Mutual solubility of acetic acid pentyl ester and water					
T/K $x_1$ $g(1)/100g sin$ (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase					
285.6	0.00030	_	0.216	-	
293.2	_	0.9565 <sup>a</sup>	-	99.375	
299.9	0.00025	-	0.180	-	
305.6	-	0.9519	-	99.306	
306.1	0.00023		0.166	-	
328.6	_	0.9318	-	98.997	
343.6	-	0.9193	-	98.800	
345.9	0.00023	-	0.166	-	
353.1	0.00025	-	0.180		
358.6	-	0.8896	-	98.312	
364.5	0.00030	-	0.216	-	
<sup>a</sup> By the Karl Fischer method. Author's smoothing equations: $x_1 = 3.583 \times 10^{-4} - 5.48 \times 10^{-6} (T/K - 273.15) + 5.22 \times 10^{-8} (T/K - 273.15)^2$ st. dev. = 3.39 x 10 <sup>-6</sup> (2)-rich phase $x_2 = 0.045710 - 3.4441 \times 10^{-4} (T/K - 273.15) + 1.267 \times 10^{-4} (T/K - 273.15)^2$ st. dev. = 3.41 x 10 <sup>-3</sup> (1)-rich phase					
		AUXILIARY :	INFORMATION		
METHOD/APP.	ARATUS/PROCEDU	RE:	SOURCE AND PURITY OF MATERIALS:		
The synthetic method of Alexejew and the analytical method were used. An ampoule with the solution of fixed concentration was placed into a glass tube connected with a thermostat filled completely with distilled water. The temperature of the bath was changed continuously			<ul> <li>(1) POCH Gliwice, pure for analysis grade; distilled; purity 99.92% by glc, 0.27 wt% water by the Karl Fischer method.</li> <li>(2) Distilled.</li> </ul>		
during the measurements and the appearance and disappearance of turbidity within the ampoule was observed visually. For the analyti- cal method, The amount of water in the saturated organic-phase was determined using a Karl Fischer titration procedure. The amount of water in the pure ester was taken into account.		ESTIMATED ERROR:			
		Temp. ±(0.2-0.6) <sup>0</sup> C. Soly. see above.			
		REFERENCES:			

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid pentyl ester	Richon, D.; Viallard, A.
(pentyl acetate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	Fluid Phase Equilib. <u>1985</u> , 21,
	279-93.
(2) water; $H_20$ ; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES:	
Mutual solubility of acet	ic acid pentyl ester and water
T/K mol(1)/	$x_1$ g(1)/100g sln (compiler)
100g(2) (2)-rich ph.	(1)-rich ph. (2)-rich ph. (1)-rich ph.
200 18 _ 2 22 × 10 <sup>-4</sup>	
$298.1^{\text{b}}$ $2.33 \times 10^{-4}$ $298.1^{\text{b}}$ $0.00144$ $2.59 \times 10^{-4}$	<sup>c</sup> – 0.1871 <sup>d</sup> –
<sup>c</sup> Compiler.	
AUXILIA	RY INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The calorimetric and differential refractometric methods were used. The calorimetric method was de- scribed in the thesis of Richon (ref 1) and by Richon and Villard (ref 2). For the refractometric measurements, a Phoenix model 1-2000T differential refractometer	<ul> <li>(1) Merck (for analysis); purified by preparation gas chromato- graphic method; purity &gt;99.5%, water content was negligible.</li> <li>(2) Distilled.</li> </ul>
from Texas Instruments was used, and the solubility was determined	ESTIMATED ERROR:
from a characteristic calibration Curve as described in the thesis o Richon (ref 1).	Soly. about $\pm 0.01^{d}$ and $\pm 0.2^{e}$ g(1)/100g sln (compiler).
	REFERENCES:
	1. Richon, D. <i>Thesis</i> , University de Clermont-Ferrand, <u>1974</u> .
	2. Richon, D.; Villard, A. <i>Can. J.</i> <i>Chem.</i> <u>1976</u> , 54, 2584.
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COMPONENTS:	ORIGINAL MEASUREMENTS:			
<pre>(1) Acetic acid pentyl ester  (pentyl acetate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;  [628-63-7]</pre>	Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.			
(2) Water; H <sub>2</sub> O; [7732-18-5]				
VARIABLES:	PREPARED BY:			
T/K = 273 - 364	Z. Maczynska			
EXPERIMENTAL VALUES: Mutual solubility of acetic acid pentyl ester and water				

t/°C	g(1)/100g sln		$x_1$ (compiler)		
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase	
0	0.29	99.21	0.00040	0.9456	
9.8	-	99.19	-	0.9443	
19.7	0.22	99.14	0.00030	0.9410	
30.6	0.16	98.78	0.00022	0.9180	
39.5	0.16	98.91	0.00022	0.9262	
50.0	0.10	98.88	0.00014	0.9243	
60.3	0.10	98.73	0.00014	0.9149	
70.2	0.17	98.63	0.00023	0.9088	
80.1	0.17	98.62	0.00023	0.9082	
90.5	-	98.46	-	0.8984	
std. de	ev. 0.01	0.02	* <u></u>		

## AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. SOURCE AND PURITY OF MATERIALS:

 Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

## ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

Сомро	NENTS:	EVALUATOR:
(1)	Butanoic acid 1-methylethyl ester ( <i>isopropyl butyrate</i> );	G.T. Hefter, School of Mathematical and Physical Sciences,
(2)	$C_{7}n_{14}O_{2}$ ; [038-11-9] Water: H_O; [7732-18-5]	Australia
(-)		January, 1989

# CRITICAL EVALUATION:

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

TABLE 1: Quantitative Solubility Studies of the Butanoic acid 1-methylethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Bomshtein et al. (ref 1)	283-363	mutual	titration
Stephenson and Stuart (ref 2)	273-363	mutual	GLC

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. SOLUBILITY OF BUTANOIC ACID 1-METHYLETHYL ESTER (1) IN WATER (2)

All the available data (ref 1,2) for the solubility of butanoic acid 1-methylethyl ester (1) in water (2) are summarized in Table 2 and plotted in Figure 1. The data are in serious disagreement differing by up to an order of magnitude. Interestingly, the data of Bomshtein *et al.* (ref 1) are lower than those reported by Stephenson and Stuart (ref 2) whereas for most other systems studied by the same authors the reverse is true. In the absence of any other studies it is not possible to prefer one data set over the other and no "Best" values are proposed, however, the data of Stephenson and Stuart (ref 2) are usually reliable. Clearly this system Warrants further investigation.

# TABLE 2: Reported Solubilities of Butanoic acid 1-methylethyl ester (1) in Water (2)

T/K	Reported solubilities	
	g(1)/100g sln	$10^3 x_1^a$
273	3.12 (ref 2)	4.4
283	0.20 (ref 1), 2.91 <sup>*</sup> (ref 2)	4.1
293	0.22 (ref 1), 2.74 <sup>*</sup> (ref 2)	3.8
298	0.24 <sup>*</sup> (ref 1), 2.67 <sup>*</sup> (ref 2)	3.8
		(continued next page)



	······			
COMPONENTS:	EVALUATOR:			
(1) Butanoic acid 1-methylethyl	G.T. Hefter, School of Mathematical			
ester ( <i>isopropyl butyrate</i> );	and Physical Sciences,			
$C_7 R_{14} U_2; [638 - 11 - 9]$	Australia			
(2) water; H <sub>2</sub> O; [//32-18-5]	January, 1989			
CRITICAL EVALUATION: (continued)	J.,			
2. SOLUBILITY OF WATER (2) IN BUTAN	DIC ACID 1-METHYLETHYL ESTER (1)			
All the available data for the so acid 1-methylethyl ester (1) are summa	olubility of water (2) in butanoic arized in Table 3 and plotted in			
Figure 2.				
Although the two studies show a p	rather different dependence on			
reasonable agreement and the average	queous phase soluplifies, are in values may be regarded as Tentative			
pending further studies.	······································			
TABLE 3: Tentat	<u>zive Solubilities</u>			
of Water (2) in Butanoic acid 1-methylethyl ester (1)				
T/K Solubilities				
Reported values	"Best" values $(\pm \sigma_n)^a$			
g(2)/100g sln	$g(2)/100g sln x_2$			
273 1.71 (ref 2)	1.7 0.11			
283 0.90 (ref 1), 1.81* (ref 2)	1.4 ± 0.5 0.09			
293 1.20 (ref 1), 1.92* (ref 2)	1.6 ± 0.4 0.11			
298 1.35* (ref 1), 2.00* (ref 2	2) 1.7 ± 0.3 0.11			
303 1.50 (ref 1), 2.06* (ref 2)	1.8 ± 0.3 0.12			
313 1.80 (ref 1), 2.20* (ref 2)	2.0 ± 0.2 0.13			
<sup>3</sup> 23 2.10 (ref 1), 2.37 <sup>*</sup> (ref 2)	2.2 ± 0.2 0.14			
333 2.30 (ref 1), 2.57* (ref 2)	2.4 ± 0.2 0.15			
343 2.60 (ref 1), 2.78* (ref 2)	2.7 ± 0.1 0.17			
353 3.40 (ref 1), 3.00 <sup>*</sup> (ref 2)	3.2 ± 0.2 0.19			
363 5.50 (ref 1), 3.20* (ref 2)	4.4 ± 1.3 0.25			

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_2)$  have the same status and (relative) percentage uncertainties as the mass solubilities.

(continued next page)





<b></b>		<u> </u>	<u></u>			
COMPONENTS:			ORIGINAL MEASUREMENTS:			
<pre>(1) Butanoic acid 1-methylethyl     ester (isopropyl butyrate);</pre>		Bomshtein, A.L.; Trofimov, A.N.; Serafimov, L.A.				
C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [638-11-9]		Zh.	Prikl. Khim.	<u>1978, 51, 1280-</u> 2	:.	
(2) Wa	ter; H <sub>2</sub> 0; [7732-1	8-5]				
VARIABLE	S:		PREP	ARED BY:		
T/K = 2	83 - 363		Α.	Skrzecz		
EXPERIME	NTAL VALUES:	- <u></u>	L			
Mut	ual solubility of	butanoic aci	id 1-m	ethylethyl es	ter and water	
t/°C	x			a(1)/100a s	ln (compiler)	
	(2)-rich phase	(1)-rich phas	se (	2)-rich phase	(1)-rich phase	
10	0.00028	0.9384		0.20	99.10	
20	0.00031	0.9193		0.22	98.80	
30	0.00035	0.9009		0.25	98,50	
40	0.00042	0.8831		0.30	98.20	
50	0.00056	0.8659		0.40	97.90	
60	0.00069	0.8547		0.50	97.70	
70	0.00091	0.8384		0.65	97.40	
80	0.00123	0.7973		0.88	96.60	
90 0.00196 0.7041			1.40	94.50		
·	<u></u>	. <u></u>	· · · · · · · · · ·			
			TNEODM			
		AUXILIARY .				
METHOD/AI	PPARATUS/PROCEDUR	Е:	SOUR	CE AND PURITY	OF MATERIALS:	
The tit: constant details	ration method was t temperature. No were reported in	used at further the paper.	(1) Source not specified; distil- led; without impurities by glc, b.p. 125.0°C, $n_D^{20}$ 1.394.		,	
			(2) Not specified.			
				-		
			PCOTI			
,			ESTIMATED ERROR:			
		Not specified.				
			REFEI	RENCES:		

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Butanoic acid 1-methylethyl ester (<i>isopropyl butyrate</i>); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>; [638-11-9]</li> <li>Water; H<sub>2</sub>O; [7732-18-5]</li> </ol>	Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.
VARIABLES:	PREPARED BY:
T/K = 273 - 363	Z. Maczynska
EXPERIMENTAL VALUES:	

Mutual solubility of butanoic acid 1-methylethyl ester and water

t/°C	/ <sup>o</sup> C g(1)/100g slr		$x_1$ (comp	mpiler)	
I	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase	
0	3.12	98.29	0.00444	0.8883	
9.7	3.08	98.13	0.00438	0.8789	
19.5	2.65	98.18	0.00375	0.8819	
30.8	2.75	97.90	0.00390	0.8658	
39.5	2.57	97.91	0.00364	0.8663	
49.7	2.49	97.70	0.00352	0.8546	
60.2	2.49	97.39	0.00352	0.8377	
70.1	2.70	97.18	0.00382	0.8266	
80.0	2.84	96.93	0.00403	0.8137	
90.2	2.98	96.85	0.00423	0.8097	
std. dev	7. 0.02	0.02			

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

# SOURCE AND PURITY OF MATERIALS:

- (1) Source not specified, commercial sample; purity 98%; used as received.
- (2) Not specified.

### ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

COMPONENTS:	EVALUATOR:
<pre>(1) Butanoic acid, 3-methyl-, ethyl ester (ethyl isovalerate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>; [108-64-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H <sub>2</sub> O; [7732-18-5]	January, 1989

#### CRITICAL EVALUATION:

Quantitative solubility data for the 3-methylbutanoic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

# TABLE 1: Quantitative Solubility Studies of the 3-Methylbutanoic acid ethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Bancroft (ref 1)	293	mutual	titration
Chang and Moulton (ref 2)	298	mutual	titration
Stephenson and Stuart (ref 3)	273-364	mutual	GLC

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. SOLUBILITY OF 3-METHYLBUTANOIC ACID ETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of 3-methylbutanoic acid ethyl ester (1) in water (2) are summarized in Table 2 except for the datum of Bancroft which is reported in v/v units and hence excluded from this Evaluation.

At 298 K, the only temperature where comparison is possible, the datum of Chang and Moulton (ref 2), is in quite good agreement with the interpolated value of Stephenson and Stuart (ref 3), lending confidence to the latter's values at other temperatures. Nevertheless, pending further studies, the data of Stephenson and Stuart must be regarded as Tentative although it may be noted that these authors' data are usually reliable.

	TABLE 2: Tentative Solubilities of 3-Methylbutanoic acid ethyl ester (1) in Water (2)		
T/K	Solubi	lities	
	Reported values	"Best" value	es <sup>a</sup>
	g(1)/100g sln	g(1)/100g sln	10 <sup>4</sup> x <sub>1</sub>
273	0.34 (ref 3)	0.3	4
283	0.24 (ref 3)	0.2	3
293	0.21 <sup>*</sup> (ref 3)	0.2	3
298	0.16 (ref 2), 0.20 <sup>*</sup> (ref 3)	0.20	2.8
		(continu	ued next page

+0			
<pre>COMPONENTS: (1) Butanoic acid, 3-methyl-,     ethyl ester     (ethyl isovalerate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;     [108-64-5] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>		EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989	
CRITI	CAL EVALUATION: (continued)		
<i>т/к</i>		Solubilities	
	Reported values	"Best" values	a
	g(1)/100g sln	g(1)/100g sln	10 <sup>4</sup> x <sub>1</sub>
303	0.19 <sup>*</sup> (ref 3)	0.2	3
313	0.17 <sup>*</sup> (ref 3)	0.2	3
323	0.16 <sup>*</sup> (ref 3)	0.2	3
333	0.16 <sup>*</sup> (ref 3)	0.2	3
343	0.16 <sup>*</sup> (ref 3)	0.2	3
353	0.16 <sup>*</sup> (ref 3)	0.2	3
363	0.16 <sup>*</sup> (ref 3)	0.2	3
a R 2. 3-me phase appli	counded values of ref 3. SOLUBILITY OF WATER (2) IN 3-M The situation with regard to the thylbutanoic acid ethyl ester and the comments under Part 1 cable and should be consulted in	ETHYLBUTANOIC ACID ETHYL EST he solubility of water (2) in (1) is identical to that of t . of this Evaluation are equa in conjunction with Table 3.	ER (1) h he H <sub>2</sub> O-rich hlly
	<u>TABLE 3: Tent</u> of Water (2) in 3-Methyl	<u>tative Solubilities</u> butanoic acid ethyl ester (1	L
T/K	1	Solubilities	
	Reported values	"Best" values	a
	g(2)/100g sln	g(2)/100g sln	$10^2 x_2$
273	0.41 (ref 3)	0.4	3
283	0.48 <sup>*</sup> (ref 3)	0.5	3
293	0.52 <sup>*</sup> (ref 3)	0.5	3
298	0.47 (ref 2), 0.61 <sup>*</sup> (ref	3) $0.54^{b}$	3.8

0.7

0.7

0.8

303

313

323

0.69<sup>\*</sup> (ref 3)

0.71<sup>\*</sup> (ref 3)

0.79<sup>\*</sup> (ref 3)

(continued next page)

5

5

COMPONENTS: (1) Butanoic acid, 3-methyl-, ethyl ester (ethyl isovalerate); $C_7H_{14}O_2$ ; [108-64-5] (2) Water; $H_2O$ ; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Ma and Physical Sciences, Murdoch University, Pert Australia January, 1989	athematical h, W.A.,
CRITICAL EVALUATION: (continued)		,
T/K Sol	lubilities	
Reported values	"Best" values	a
g(2)/100g sln	g(2)/100g sln	$10^2 x_2$
333 0.83 <sup>*</sup> (ref 3)	0.8	6
343 0.85 <sup>*</sup> (ref 3)	0.9	6
353 0.94 <sup>*</sup> (ref 3)	0.9	6
363 1.11 <sup>*</sup> (ref 3)	1.1	8
<sup>b</sup> Average value. REFERENCES	2 114-26	
1. Bancroft, W. D. Phys. Rev. <u>1895</u> ,	3, 114-36.	
<ul> <li>Chang, Y. C.; Moulton, R. W. Ind. Eng. Chem. <u>1953</u>, 45, 2350-61.</li> <li>Stophonson R.: Stuart T. J. Chem. Eng. Data 1986, 31, 56, 70</li> </ul>		50-61.
<ol> <li>Bancroft, W. D. Phys. Rev. <u>1895</u>, 3, 114-36.</li> <li>Chang, Y. C.; Moulton, R. W. Ind. Eng. Chem. <u>1953</u>, 45, 2350-61.</li> <li>Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u>, 31, 56-70.</li> </ol>		

<pre>COMPONENTS: (1) Butanoic acid, 3-methyl-,     ethyl ester         (ethyl isovalerate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;         [108-64-5] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Bancroft, W.D. Phys. Rev. <u>1895</u> , 3, 114-36.
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of 3-methylbutanoic ac reported to be 0.02 mL(1)/10mL(2). The solubility of water in 3-methylbu reported to be 0.04 mL(2)/10mL(1).	cid ethyl ester in water at 20°C was
AUXTLTARY	INFORMATION
The titration method was used. 10 mL of solvent in a test tube was titrated with the second component until the solution became cloudy.	<ul> <li>(1) Laboratory source; dried over CaCl<sub>2</sub>, distilled.</li> <li>(2) Not specified.</li> </ul>
	ESTIMATED ERROR:
	Soly. ±0.01 mL.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Butanoic acid, 3-methyl-,	Chang, Yi-C.; Moulton, R.W.	
ethyl ester	Ind. Eng. Chem. 1953, 45, 2350-61.	
$(ethyl isovalerate); C_7H_{14}O_2;$	,,,	
(2) water; H <sub>2</sub> 0; [//32-18-5]		
VARIABLES:	PREPARED BY:	
$\pi/\kappa = 298$	A Skrzecz	
EXPERIMENTAL VALUES: The solubility of 3-methylbutanoic acid ethyl ester in water at $25^{\circ}$ C w reported to be 0.16 g(1)/100g(2). The corresponding mass per cent and fraction, $x_1$ , values calculated by the compiler are 0.16 g(1)/100g sln 2.2 x $10^{-4}$ . The solubility of water in 3-methylbutanoic acid ethyl ester at $25^{\circ}$ C w reported to be 0.47 g(2)/100g(1). The corresponding mass per cent and fraction, $x_2$ , values calculated by the compiler are 0.47 g(2)/100g sln 0.033.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. The 100g portion of solvent in a ther- mostated container was titrated with the second component from a 1 mL pipette calibrated to 0.01 mL. An average of two closest values (definitely cloud and definitely clear) was presented. The amount of solute (about 0.2 mL) was very dif- ficult to judge and it was accurate only to 0.05 mL. The data were re- ported together with the ternary system 3-methylbutanoic acid ethyl ester-water-benzene.	<ul> <li>(1) Source not specified; washed with dilute KOH and H<sub>2</sub>O, de- hydrated with anhydrone, fractionally distilled; purity 99.8% by a saponifi- cation test, b.p. range 133-134°C at 755 mm Hg, n<sub>D</sub><sup>20</sup> 1.3968.</li> <li>(2) Distilled (distillation from KMnO<sub>4</sub> caused no change in the refractive index).</li> <li>ESTIMATED ERROR: Temp. ±0.1°C. Soly. ±25% (probably relative error).</li> <li>REFERENCES:</li> </ul>	

52				
COMPONENTS: (1) Butanoic acid, 3-methyl-, ethyl ester (ethyl isovalerate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [108-64-5]		ORIGINAL MEASUREMEN Stephenson, R.; St J. Chem. Eng. Data 56-70.	NTS: cuart, J. a <u>1986</u> , 31,	
(2) Water;	H <sub>2</sub> 0; [7732-	18-5]		
VARIABLES:			PREPARED BY:	
T/K = 273 -	364		Z. Maczynska	
EXPERIMENTAL Mutual s	VALUES: olubility o	of 3-methylbuta	anoic acid ethyl este	er and water
t/°C (2)	g(1)/1 -rich phase	.00g sln 2 (1)-rich phas	x <sub>1</sub> (compi se (2)-rich phase	ler) (1)-rich phase
0 9.0 19.4 30.6 39.8 49.5 60.1 70.0 80.3 90.5 std. dev.	0.34 0.22 0.20 0.17 0.16 0.15 0.16 0.16 0.16 0.16	99.588 99.527 99.442 99.355 99.293 99.211 99.173 99.155 99.057 98.877 0.004	0.00047 0.00033 0.00028 0.00023 0.00022 0.00021 0.00022 0.00022 0.00022 0.00022	0.97097 0.96679 0.95103 0.95519 0.95106 0.94565 0.94316 0.94199 0.93563 0.92415
		AUXILIARY :	INFORMATION	
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.		SOURCE AND PURITY C (1) Source not spe cial sample; p as received. (2) Not specified. ESTIMATED ERROR: Accuracy of method for solubility, se REFERENCES:	oF MATERIALS: cified, commer- ourity 99%; used 0.1 wt% or less, e above.	

COMPONENTS:		EVALUATOR:
(1)	Butanoic acid propyl ester ( <i>propyl butyrate</i> ); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [105-66-8]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia January, 1989

# CRITICAL EVALUATION:

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

TABLE 1: Quantitative Solubility Studies of the Butanoic acid propyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Fuehner (ref 1)	290	(1) in (2)	titration
Stephenson and Stuart (ref 2)	273-364	mutual	GLC

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. SOLUBILITY OF BUTANOIC ACID PROPYL ESTER (1) IN WATER (2)

All the available data are summarized in Table 2. At 290 K, the only temperature where comparison is possible, the values of Fuehner (ref 1) and Stephenson and Stuart (ref 2) are in good agreement giving confidence in the remaining data of ref 2. However, in the absence of independent studies the data of Stephenson and Stuart must be regarded as Tentative although it may be noted that the solubilities of these authors are usually reliable.

<u>TABLE 2: Tentative Solubilities</u> of Butanoic acid propyl ester (1) in Water (2)			
T/K	Solubil	lities	
	Reported values	"Best" value	es <sup>a</sup>
	g(1)/100g sln	g(1)/100g sln	$10^4 x_1$
273	0.30 (ref 2)	0.3	4
283	0.22 <sup>*</sup> (ref 2)	0.2	3
290	0.162 (ref 1), 0.19 <sup>*</sup> (ref 2)	0.18	2.5
293	0.19 <sup>*</sup> (ref 2)	0.2	3
298	0.18 <sup>*</sup> (ref 2)	0.2	3
303	0.17 <sup>*</sup> (ref 2)	0.2	3
****	······	(contin	ued next page

COMPONENTS:		EVALUATOR:
<pre>(1) Butanoic acid propyl ester (propyl butyrate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;</pre>		G.T. Hefter, School of Mathematical and Physical Sciences,
(2)	[105-66-8] Water; H <sub>2</sub> O; [7732-18-5]	Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K		Solubilit	ies	
		Reported values	"Best" values <sup>a</sup>	
		g(1)/100g sln	g(1)/100g sln	10 <sup>4</sup> x <sub>1</sub>
313	0.16*	(ref 2)	0.2	3
323	0.16*	(ref 2)	0.2	3
333	0.16*	(ref 2)	0.2	3
343	0.16*	(ref 2)	0.2	3
353	0.16*	(ref 2)	0.2	3
363	0.16*	(ref 2)	0.2	3

<sup>a</sup> Rounded values of ref 2 except at 290 K.

2. SOLUBILITY OF WATER (2) IN BUTANOIC ACID PROPYL ESTER (1)

Only the data of Stephenson and Stuart (ref 2) are available for the solubility of water (2) in propyl butyrate (1) and so no Critical Evaluation is possible. The interested user is referrd to the relevant Data Sheet for the experimental solubilities but it may be noted that the data of Stephenson and Stuart (ref 2) are usually reliable.

- 1. Fuehner, H. Ber. Dtsch. Chem. Ges. <u>1924</u>, 57, 510-5.
- 2. Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u>, 31, 56-70.

<b></b>		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Butanoic acid propyl ester	Fuehner, H.	
(propyl butyrate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	Ber. Dtsch. Chem. Ges. <u>1924</u> , 57 510-5	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 290	A. Skrzecz	
	A. DA12002	
EXPERIMENTAL VALUES: The solubility of butanoic acid propy to be 0.195 vol%, 0.162 g(1)/100g slr sponding mole fraction, $x_1$ , value cal 2.24 x 10 <sup>-4</sup> .	vl ester in water at 17 <sup>°</sup> C was reported h and 0.0124 mol(1)/L sln. The corre- culated by the compiler is	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. The ester was added from pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remain- ed transparent.	<ul><li>(1) Source not specified, commer- cial product.</li><li>(2) Not specified.</li></ul>	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

56					
COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Butanoic acid propyl ester			Stephenson, R.; Stuart, J.		
( <i>propyl butyrate</i> ); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [105-66-8]			J. Chem. Eng. Data <u>1986</u> , 31, 56-70.		
(2) Water	; H <sub>2</sub> O; [7732-	18-5]			
VARIABLES:			PREPARED BY:		
T/K = 273 - 364			Z. Maczynska		
EXPERIMENTA Mut	AL VALUES: ual solubilit	y of butanoic	acid propyl ester a	nd water	
$t/^{\circ}$ C g(1)/100g sln $x_1$ (compiler) (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase					
0	0.30	99.36	0.00042	0,9555	
9.6	0.23	-	0.00032	-	
20.1	0.19	99.37	0.00026	0.9562	
29.6	0,15	99.36	0.00021	0.9555	
39.5	0.14	99.34	0.00019	0.9542	
49.8	0.17	99.16	0.00023	0.9423	
60.1	0.21	98.52	0.00029	0.9021	
70.1	0.15	-	0.00021	-	
80.1	0.14	99.01	0.00019	0.9326	
90.5	0.17	98.19	0.00023	0.8824	
std. dev.	0.01	0.01			
<u> </u>		AUXILIARY	INFORMATION		
			SOURCE AND PURITY (	OF MATERIALS:	
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.			<ul> <li>(1) Source not specified, commer- cial sample; purity 99%; used as received.</li> <li>(2) Not specified.</li> </ul>		
			ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above.		
			REFERENCES:		

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COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Formic acid hexyl ester			Stephenson, R.; Stuart, J.			
(hexyl formate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;			J. Chem. Eng. Data 1986. 31.			
[629-33-4]			56-70.			
(2) Water; H <sub>2</sub> O; [7732-18-5]						
VARIABLES:			PREPARED BY:			
T/K = 273 - 364			Z. Maczynska			
EXPERIME	NTAL VALUES:					
	Mutual solubili	cy of formic a	cid hex	/I ester and		
t/°C	g(1)/10	00g sln		$x_1$ (comp	oiler)	
	(2)-rich phase	(1)-rich phas	e (2)·	-rich phase	(1)-rich phase	
0	-	99.474			0.96319	
8.7	0.17	99.475		0.00024	0.96326	
19.7	0.15	99.492		0.00021	0.96441	
29.7	0.13	99.401		0.00018	0.95826	
39.6	0.13	99.340		0.00018	0.95418	
49.8	0.11	99.346		0.00015	0.95458	
60.2	0.11	99.281		0.00015	0.95027	
70.3	0.12	-		0.00017	-	
80.2	0.13	99.153		0.00018	0.94185	
90.6	0.14	99.201		0.00019	0.94499	
std. d	dev. 0.01	0.003				
		AUXILIARY I	NFORMAT	ION		
METHOD/AF	PPARATUS/PROCEDU	<b>λΕ:</b>	SOURCE	AND PURITY	OF MATERIALS:	
The anal	lytical method wa	is used.	(1) Source not specified, commer-			
Componer With com	nt (1) was equili popent (2) at a	brated given	ci as	al sample; received.	purity 96%; used	
temperat	ure in a thermos	stat. Each	(2) Not specified.			
layer wa (1) was	is sampled with a determined by ad	l syringe; Iding a				
weighed	amount of acetor	itrile				
(or some organic	etimes propanol) laver sample and	to the I measuring				
by a Gow-Mac thermal conductivity			ESTIMAT	ED ERROR:		
gc the ( (Chromos	gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).			Accuracy of method 0.1 wt% or less, for solubility, see above.		
3390 A r						
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.						
			REFERENCES:			
		j				

COMPONENTS:	ORIGINAL MEASUREMENTS:				
<pre>(1) Hexanoic acid methyl ester (methyl caproate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>; [106-70-7]</pre>	Stephenson, R.; Stuart, J. <i>J. Chem. Eng. Data</i> <u>1986</u> , 31, 56-70.				
(2) Water; H <sub>2</sub> O; [7732-18-5]					
VARIABLES:	PREPARED BY:				
T/K = 273 - 364	Z. Maczynska				
EXPERIMENTAL VALUES: Mutual solubility of hexanoic acid methyl ester and water					

t∕°C	g(1)/10	g(1)/100g sln		x <sub>1</sub> (compiler)		
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase		
0	0.241	99.62	0.000334	0.9732		
9.3	0.177	99.54	0.000245	0.9677		
20.0	0.166	99.45	0.000230	0.9616		
29.7	0.167	99.40	0.000231	0.9582		
39.5	0.129	99.32	0.000179	0.9528		
50.0	0.137	99.25	0.000190	0.9482		
60.0	0.132	99.19	0.000183	0.9442		
70.2	0.128	99.20	0.000177	0.9449		
80.2	0.138	99.17	0.000191	0.9429		
90.5	0.147	99.11	0.000204	0.9390		
std. dev	v. 0.001	0.01				

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

# SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial sample; purity 99%; used as received.
- (2) Not specified.

## ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.
COMPONENTS:		EVALUATOR:	
(1)	Pentanoic acid ethyl ester (ethyl valerate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,	
	[539-82-2]	Murdoch University, Perth, W.A.,	
(2)	Water: H <sub>2</sub> O: [7732-18-5]	Australia	
`-'		January, 1989	

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

TABLE 1: Quantitative Solubility Studies of the Pentanoic acid ethyl ester (1) - Water (2) System

Reference	9	T/K	Solubility	Method
Hemptinne (ref 1)		298	(1) in (2)	analytical
Bomshtein et al. (1	cef 2)	283-353	mutual	titration

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. SOLUBILITY OF PENTANOIC ACID ETHYL ESTER (1) IN WATER (2)

For the solubility of pentanoic acid ethyl ester (1) in water (2) all the available data are summarized in Table 2. At 298 K, the only temperature where comparison is possible, the datum of Hemptinne (ref 1) is in good agreement with the interpolated value of Bomshtein *et al.* (ref 2). However, it should be noted that the solubilities reported by Bomshtein *et al.* often differ significantly from the "Best" values in well-characterized systems. For this reason the data in Table 2 should be regarded as very Tentative.

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COMPONENTS:	EVALUATOR:
(1) Pentanoic acid ethyl ester	G.T. Hefter, School of Mathematical
(ethyl valerate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	and Physical Sciences,
[539-82-2]	Australia
(2) Water; H <sub>2</sub> O; [7732-18-5]	January, 1989

# TABLE 2: Tentative Solubilities of Pentanoic acid ethyl ester (1) in Water (2)

T/K	Solubilities				
	Reported values	"Best" values <sup>a</sup>			
	g(1)/100g sln	g(1)/100g sln	$10^4 x_1$		
283	0.24 (ref 2)	0.2	3		
293	0.25 (ref 2)	0.25	3.5		
298	0.237 (ref 1), 0.255 <sup>*</sup> (ref 2)	0.25	3.5		
303	0.26 (ref 2)	0.3	4		
313	0.27 (ref 2)	0.3	4		
323	0.32 (ref 2)	0.3	4		
333	0.37 (ref 2)	0.4	6		
343	0.55 (ref 2)	0.6	8		
353	0.78 (ref 2)	0.8	11		

<sup>a</sup> Rounded values of ref (2), but see text.

2. SOLUBILITY OF WATER (2) IN PENTANOIC ACID ETHYL ESTER (1)

As the only data available for the solubility of water (2) in pentanoic acid ethyl ester (1) are those of Bomshtein *et al.* (ref 2) no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet but the comments made under part 1. of this Evaluation above should be noted.

### REFERENCES

1. Hemptinne, A. Z. Phys. Chem. <u>1894</u>, 13, 561-9.

 Bomshtein, A. L.; Trofimov, A. N.; Serafimov, L. A. Zh. Prikl. Khim. <u>1978</u>, 51, 1280-2.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) Pentanoic acid ethyl ester (ethyl valerate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>; [539-82-2]</pre>	Hemptinne, A. Z. Phys. Chem. <u>1894</u> , 13, 561-9.		
(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 298	A. Skrzecz		

EXPERIMENTAL VALUES:

The solubility of pentanoic acid ethyl ester in water at  $25^{\circ}C$  was reported to be 2.366 g(1)/L sln.

No	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The mixture of water with excess ester was heated for some time in a water bath and the ester phase was filtered. A sample of known volume was then transferred to a smaller flask, heated with the known amount of baryta until complete saponifi- cation was obtained and then ti- trated. No further details were reported in the paper.	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:

	rs:		ORIGINAL MEASUREMENTS:			
<ul> <li>(1) Pentanoic acid ethyl ester (ethyl valerate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>; [539-82-2]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> <li>VARIABLES: T/K = 283 - 353</li> </ul>			Bomshtein, A.L.; Serafimov, L.A.	Bomshtein, A.L.; Trofimov, A.N.; Serafimov, L.A. Zh. Prikl. Khim. <u>1978</u> , 51, 1280-2.		
			Zh. Prikl. Khim.			
			PREPARED BY:			
			A. Skrzecz			
(PERIME)	NTAL VALUES:					
1	Mutual solubilit	y of pentanoi	c acid ethyl ester a	and water		
t/°C		x_1	g(1)/100g sl	n (compiler)		
	(2)-rich phase	(1)-rich pha	se (2)-rich phase	(1)-rich phase		
10	0.00033	0.9928	0.24	99.90		
20	0.00034	0.9650	0.25	99.50		
30	0.00036	0.9257	0.26	98.90		
40	0.00038	0.9009	0.27	98.50		
50	0.00044	0.8715	0.32	98.00		
60	0.00051	0.8492	0.37	97.60		
70	0.00077	0.8226	0.55	97.10		
80	0.00109	0.7828	0.78 96.30			
<u></u>				<u></u>		
		AUXILIARY	INFORMATION			
THOD/AH	PPARATUS/PROCEDU	AUXILIARY RE:	INFORMATION SOURCE AND PURITY	OF MATERIALS:		
THOD/AN he titr onstant letails	PPARATUS/PROCEDU cation method wa t temperature. N were reported i	AUXILIARY RE: s used at o further n the paper.	INFORMATION SOURCE AND PURITY (1) Source not sp led; without b.p. 145.2°C, (2) Not specified	OF MATERIALS: pecified; distil- impurities by glo $n_D^{20}$ 1.400.		
THOD/AH he titr onstant letails	PPARATUS/PROCEDU cation method wa temperature. N were reported i	AUXILIARY RE: s used at o further n the paper.	INFORMATION SOURCE AND PURITY (1) Source not sp led; without b.p. 145.2°C, (2) Not specified	OF MATERIALS: pecified; distil- impurities by glo $n_D^{20}$ 1.400.		
THOD/AI he titr onstant letails	PPARATUS/PROCEDU ration method wa t temperature. N were reported i	AUXILIARY RE: s used at o further n the paper.	INFORMATION SOURCE AND PURITY (1) Source not sp led; without b.p. 145.2°C, (2) Not specified ESTIMATED ERROR:	OF MATERIALS: pecified; distil- impurities by glo $n_D^{20}$ 1.400.		
THOD/AI he titr onstant letails	PPARATUS/PROCEDU ration method wa temperature. N were reported i	AUXILIARY RE: s used at o further n the paper.	INFORMATION SOURCE AND PURITY (1) Source not sp led; without b.p. 145.2°C, (2) Not specified ESTIMATED ERROR: Not specified.	OF MATERIALS: pecified; distil- impurities by glo n <sub>D</sub> <sup>20</sup> 1.400.		

COMPONENTS:		EVALUATOR:					
<ul> <li>(1) Propanoic acid butyl est (butyl propionate); C<sub>7</sub>H<sub>1</sub> [590-01-2]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	ter <sub>14</sub> 0 <sub>2</sub> ; ]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989					
CRITICAL EVALUATION:							
Quantitative solubility data for the propanoic acid butyl ester (1) - water (2) system have been reported in the publications listed in Table 1. <u>TABLE 1: Quantitative Solubility Studies of the</u> <u>Propanoic acid butyl ester (1) - Water (2) System</u>							
Reference	T/K	Solubility	Method				
Bridgman (ref 1) 280-303 (2) in (1) synthetic							
Park and Hopkins (ref 2) 298 (1) in (2) unspecified							
Doolittle (ref 3)	293	mutual	unspecified				
Bomshtein et al. (ref 4)	368	mutual	titration				
Stephenson and Stuart (ref 5)	273-364	mutual	GLC				

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. SOLUBILITY OF PROPANOIC ACID BUTYL ESTER (1) IN WATER (2)

Apart from the single temperature values of Doolittle (ref 3) and Bomshtein et al. (ref 4), only the data of Stephenson and Stuart (ref 5) are available for the solubilities of propanoic acid butyl ester (1) in water (2) over a range of temperatures. The datum of Doolittle (ref 3) is in reasonable agreement with that of Stephenson and Stuart (ref 5) but Bomshtein et al.'s (ref 4) value is an order of magnitude higher. In the absence of confirmatory studies it is not possible to assess the quality of these data although it may be noted that the data of Stephenson and Stuart (ref 5) are generally reliable and those of Bomshtein et al. (ref 4) are often high.

COMPC	DNENTS:	EVALUATOR:
(1)	Propanoic acid butyl ester	G.T. Hefter, School of Mathematical
	(590-01-2]	Murdoch University, Perth, W.A.,
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia
		January, 1989

	TABLE	2:	Repor	ted So	<u>lubi</u>	<u>lities</u>	
<u>of</u>	Propanoic	acid	butyl	ester	(1)	in Water	(2)

T/K	Reported Solubilities	
	g(1)/100g sln	10 <sup>4</sup> x <sub>1</sub> <sup>a</sup>
273	0.298 (ref 5)	4.1
283	0.228 <sup>*</sup> (ref 5)	3.2
293	0.15 (ref 3), 0.193 <sup>*</sup> (ref 5)	2.7
298	0.180 <sup>*</sup> (ref 5)	2.5
303	0.169 <sup>*</sup> (ref 5)	2.3
313	0.155 <sup>*</sup> (ref 5)	2.1
323	0.146 <sup>*</sup> (ref 5)	2.0
333	0.143 <sup>*</sup> (ref 5)	2.0
343	0.141 <sup>*</sup> (ref 5)	1.9
353	0.142 <sup>*</sup> (ref 5)	2.0
363	$1.4^{b}$ (ref 4), $0.142^{*}$ (ref 5)	2.0

<sup>a</sup> Data of Stephenson and Stuart (ref 5).

<sup>b</sup> 368 K (boiling point of mixture).

2. SOLUBILITY OF WATER (2) IN PROPANOIC ACID BUTYL ESTER (1)

All the available data for the solubility of water (2) in propanoic acid butyl ester (1) are summarized in Table 3. The situation for the organic-rich phase is better than for the aqueous phase, with the values of Bridgman (ref 1) being in excellent agreement with those of Stephenson and Stuart (ref 5) from 283-303 K. At other temperatures only the data of Stephenson and Stuart are available and in the absence of confirmatory studies must be regarded as Tentative.

COMPONENTS:	EVALUATOR:			
<ul> <li>(1) Propanoic acid butyl ester</li> <li>(butyl propionate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;</li> <li>[590-01-2]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia			
	January, 1989			
CRITICAL EVALUATION: (continued)				
<u>TABLE 3: Recommended (R) and Tentative Solubilities</u> of Water (2) in Propanoic acid butyl ester (1)				
T/K Sol	lubilities			
Reported values	"Best" values $(\pm \sigma_n)^a$			
g(2)/100g sln	$g(2)/100g sln 10^2 x_2$			
273 0.48 (ref 5)	0.5 4			
283 0.470 <sup>*</sup> (ref 1), 0.53 <sup>*</sup> (ref	5) 0.50 ± 0.03 (R) 3.5			
293 0.546 <sup>*</sup> (ref 1), 0.80 <sup>b</sup> (ref 0.62 <sup>*</sup> (ref 5)	3), 0.58 ± 0.04 (R) 4.0			
298 0.606 <sup>*</sup> (ref 1), 0.68 <sup>*</sup> (ref	5) 0.64 ± 0.04 (R) 4.5			
303 0.686 (ref 1), 0.73* (ref 5	) $0.71 \pm 0.02$ (R) 4.9			
313 0.82 <sup>*</sup> (ref 5)	0.8 6			
323 0.86 <sup>*</sup> (ref 5)	0.9 6			
333 0.89* (ref 5)	0.9 6			
343 0.92* (ref 5)	0.9 6			
353 0.94 <sup>*</sup> (ref 5)	0.9 6			
363 3.76 <sup>c</sup> (ref 4), 1.00 <sup>*</sup> (ref 5)	) 1.0 7			
<sup>a</sup> Obtained by averaging where appropriate; $\sigma_n$ has no statistical significance. Mole fraction solubilities $(x_2)$ have the same status and (relative) percentage uncertainties as the mass % solubilities. <sup>b</sup> Not included in calculation of "Best" value, see text. <sup>c</sup> 368 K; not included in calculation of "Best" value, see text.				
REFERENCES				
1. Bridgman, J. A. Ind. Eng. Chem.	<u>1928</u> , 20, 184-7.			
2. Park, J. G.; Hopkins. M. B. Ind	. Eng. Chem. <u>1930</u> , 22, 826-30.			
3. Doolittle, A. K. Ind. Eng. Chem.	<u>1935</u> , 27, 1169-79.			
<ol> <li>Bomshtein, A. L.; Trofimov, A. N Zh. Prikl. Khim. <u>1984</u>, 57, 18-23.</li> </ol>	Bomshtein, A. L.; Trofimov, A. N.; Serafimov, L. A. Zh. Prikl. Khim. <u>1984</u> , 57, 18-23.			
5. Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.				

F		I
COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Propanoic acid butyl ester		Bridgman, J.A.
(butyl propionate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;		Ind. End. Chem. <u>1928</u> , 20, 184-7.
[590-01-2]		
(2) Water; $H_20$ ; [7732-18-	-5]	
VARIABLES:		PREPARED BY:
T/K = 280 - 303		Z. Maczynska
EXPERIMENTAL VALUES:		J
Solubility of wat	er in propar	noic acid butyl ester
t/°C g(2)/100g(1)	g(2)/10	$00g$ solution $x_2$
	(cc	ompiler) (compiler)
7.0 0.452	0	0.450 0.0316
22.5 0.576	r	0.573 0.0400
30.0 0.691	c	0.686 0.0475
- 		
<u></u>	AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE	:	SOURCE AND PURITY OF MATERIALS:
The synthetic method simil that described by Groschur was used. A glass tube of 100 mL capacity with a sto filled with weighed (1) an shaking the tube after it warmed somewhat, the water solved completely in the of ter which the tube was pla 2-liter beaker filled with and equipped with an agita alternate slow cooling and it was possible to determin in about 0.5°C, the temper which water was precipitat the solution, as shown by clouding of the liquid whi clear again when the temper was slightly increased.	lar to ff (ref 1) about ppcock was had been r was dis- ester, af- aced in a n water ator. By d warming, ine, with- rature at ced from the ich would erature	<pre>(1) Source not specified; distil- led; b.p. range 144-146°C; boiled for some time in open flask before used. (2) Not specified. ESTIMATED ERROR: Temp. ±0.25°C. REFERENCES: 1. Groschuff, E. Z. Elektrochem. 1911, 17, 348.</pre>

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Propanoic acid butyl ester   (butyl propionate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;   [590-01-2]</pre>	Park, J.G.; Hopkins, M.B. Ind. Eng. Chem. <u>1930</u> , 22, 826-30.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES:	
I the solubility of propanoic acid buty	'i ester in water at 25°C was reported

to be 0.2 mL(1)/100mL(2).

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Source not specified, commer- cial samples; used as received.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Propanoic acid butyl ester	Doolittle, A.K.	
(butyl propionate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ;	Ind. End. Chem. <u>1935</u> , 27, 1169-79.	
[590-01-2]		
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES:		
The solubility of propanoic acid butyl ester in water at 20 <sup>0</sup> C was reporte		
to be 0.15 g(1)/100g sln. The corresp	bonding mole fraction, $x_1$ , value cal-	
culated by the compiler is 2.1 x 10 <sup>-4</sup>	•	
The solubility of water in propanoic	acid butyl ester at 20°C was reported	
to be 0.80 g(2)/100g sln. The corresp	bonding mole fraction, $x_2$ , value cal-	
culated by the compiler is 0.055.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Source not specified, commer- cial product; purity 99%, b.p.	
	range 124-171°C, $d_4^{20}$ 0.874.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

<b>-</b>	••••••••••••••••••••••••••••••••••••••	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Propanoic acid butyl ester   (butyl propionate); C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>;</pre>	Bomshtein, A.L.; Trofimov, A.N.; Serafimov, L.A.	
[590-01-2]	Zh. Prikl. Khim. <u>1984</u> , 57 18-23.	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 368	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of propanoic acid butyl ester in water at 94.8°C <sup>a</sup> was re- ported to be $x_1 = 0.002$ . The corresponding mass per cent value calculated by the compiler is 1.4 g(1)/100g sln. The solubility of water in propanoic acid butyl ester at 94.8°C <sup>a</sup> was re- ported to be $x_2 = 0.220$ . The corresponding mass per cent value calculated by the compiler is 3.76 g(2)/100g sln. <sup>a</sup> Boiling temperature at 101.32 kPa.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. The data and method were reported to- gether with the ternary system propanoic acid butyl ester-water- acetic acid. No further details were reported in the paper.	<ul> <li>(1) Source not specified; distilled; without impurities by glc, b.p. 145.3°C, n<sub>D</sub><sup>20</sup> 1.4011.</li> <li>(2) Not specified.</li> </ul>	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

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COMPONENTS:		ORIGINAL MEASUREME	NTS:	
(1) Propanoic acid butyl ester		Stephenson, R.; S	tuart, J.	
(butyl propionate); C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [590-01-2]		J. Chem. Eng. Dat 56-70.	a <u>1986</u> , 31,	
(2) Wat	er; H <sub>2</sub> O; [7732-1	.8-5]		
VARIABLES	:		PREPARED BY:	
T/K = 27	3 - 364		Z. Maczynska	
EXPERIMENTAL VALUES:		<u> </u>		
М	utual solubility	v of propanoic	acid butyl ester a	and water
t/°C g(1)/100g sln		$x_1$ (comp	iler)	
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase
0	0.298	99.52	0.000413	0.9663
9.4	0.230	99.47	0.000319	0.9629
19.8	0.197	99.38	0.000273	0.9568
30.6	0.167	99.14	0.000231	0.9410
40.2	0.144	99.15	0.000199	0.9417
50.0	0.146	99.15	0.000202	0.9417
59.9	0.142	99.11	0.000197	0.9390
70.1	0.140	99.08	0.000194	0.9371
80.2	0.147	99.07	0.000204	0.9365
90.4	0.142	99.00	0.000197	0.9320
std. d	ev. 0.003	0.01		
, , , , , , , , , , , , , , , , ,		AUXILIARY 1	INFORMATION	
METHOD/AP	PARATUS/PROCEDUF	E:	SOURCE AND PURITY	OF MATERIALS:
The analy	vtical method wa	s used	(1) Source not sn	ecified commer-
Componen	t (1) was equili	brated	cial sample;	purity 99%; used
temperat	ponent (2) at a ure in a thermos	given stat. Each	as received.	
layer wa	s sampled with a	syringe;	(2) Not specified	
(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol)				
		ESTIMATED ERROR:		
		Accuracy of metho	d 0.1.wt% or less,	
		for solubility, s	ee above.	
was used to determine (2) in the				
water layer.		REFERENCES:		
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COMPONENTS:		ORIGINAL MEASUREMENT	s:	
(1) Propanoic acid,		Stephenson, R.: Stu	artT.	
2,2-dimethyl-, ethyl ester				
(ethyl trimethylacetate);		J. Chem. Eng. Data 56-70,	<u>1986</u> , 31,	
C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> ; [3938-95-2]				
(2) Wat	er; H <sub>2</sub> O; [7732-	18-5]		
VARIABLES:		PREPARED BY:	· · · · · · · · · · · · · · · · · · ·	
T/K = 27	73 - 364		Z. Maczynska	
EXPERIMENTAL VALUES:		I		
Mutual	solubility of	2,2-dimethylp	copanoic acid ethyl es	ter and water
t/°C	g(1)/1	00g sln	x <sub>1</sub> (compile	 ≥r)
	(2)-rich phase	(1)-rich phas	se (2)-rich phase (1	)-rich phase
0	0.304	99.65	0.000422	0.9752
9.5	0.298	99.57	0.000413	0.9697
20.0	0.183	99.49	0.000253	0.9643
30.7	0.168	99.39	0.000233	0.9575
40.1	0.135	99.33	0.000187	0.9535
50.0	0.152	99.29	0.000210	0.9508
60.2	0.126	99.24	0.000174	0.9475
70.3	0.120	99.22	0.000166	0.9462
80.4	0.124	99.18	0.000172	0.9436
90.4	0.112	99.19	0.000155	0.9443
std. dev. 0.004 0.01				
		AUXTLIARY	INFORMATION	·
METHOD/AP	PARATUS/PROCEDU	KE:	SOURCE AND PURITY OF	MATERIALS:
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (a g theyapol)		<ol> <li>Source not speci cial sample; pur as received.</li> </ol>	fied, commer- ty 98%; used	
		(2) Not specified.		
		ESTIMATED ERROR:		
		Accuracy of method ( for solubility, see	).1 wt% or less, above.	
Was used to determine (2) in the Water layer.		REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid 3-methoxy-1-butyl	Doolittle, A.K.	
acetate): C-H14O2: [4435-53-4]	Ind. End. Chem. <u>1935</u> , 27, 1169-79.	
(2) Water: $H_{2}O$ : [7732-18-5]		
VADTABLES.	DREDARED BV.	
	A Skygoog	
17K - 293	A. 5AI 2002	
EXPERIMENTAL VALUES:		
The solubility of acetic acid 3-metho	pxy-1-butyl ester in water at 20°C was	
reported to be 6.46 g(1)/100g sln. Th	the corresponding mole fraction, $x_1$ ,	
value calculated by the compiler is (	0.00844.	
The solubility of water in acetic aci	d 3-methoxy-1-butyl ester at 20°C was	
reported to be 3.72 g(2)/100g sln. Th	ne corresponding mole fraction, $x_2$ ,	
value calculated by the compiler is (	0.239.	
AUXILIARY :	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Source not specified,	
	commercial product; purity 99%, b.p. range $135-173^{\circ}$ C, $d_4^{20}$ 0.956.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid, 2-hydroxy-,	Doolittle, A.K.
1-butyl ester (butyl lactate);	Ind. End. Chem. <u>1935</u> , 27, 1169-79.
C <sub>7</sub> H <sub>14</sub> O <sub>3</sub> ; [138-22-7]	
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES:	1
The solubility of 2-hydroxypropanoic	acid 1-butyl ester in water at 20°C
was reported to be 4.0 g(1)/100g sln.	. The corresponding mole fraction, $x_1$ ,
value calculated by the compiler is (	0.0051.
The solubility of water in 2-hydroxy	propanoic acid 1-butyl ester at 20°C
was reported to be $14.5 g(2)/100g slr$	n. The corresponding mole fraction,
$x_2$ , value calculated by the compiler	is 0.579.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commercial product; purity 97%, b.p. range 145-230°C, d <sub>4</sub> <sup>20</sup> 0.980.
	(2) Not specified.
	ESTIMATED ERROR.
	Not enocified
	Not specified.
	REFERENCES:

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ORIGINAL MEASUREMENTS: Richon, D.; Viallard, A. <i>Fluid Phase Equilib.</i> <u>1985</u> , 21, 279-93.		
PREPARED BY:		
A. Skrzecz		
EXPERIMENTAL VALUES: The solubility of acetic acid phenyl ester in water at 298.1 K was reported to be 0.00416 mol(1)/100 g(2). The corresponding mass per cent and mole fraction, $x_1$ , values calculated by the compiler are 0.558 g(1)/100g sln and 7.42 x 10 <sup>-4</sup> .		
INFORMATION		
<pre>SOURCE AND PURITY OF MATERIALS: (1) Merck (for synthesis); purified by preparation gas chromato- graphic method; purity &gt;99.5%, water content was negligible. (2) Distilled. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES: 1. Richon, D. Thesis, University de Clermont-Ferrand, 1974.</pre>		

COMPONENTS:		EVALUATOR:	
(1)	Benzoic acid methyl ester (methyl benzoate); C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematica and Physical Sciences,	
	[93-58-3]	Murdoch University, Perth, W.A.,	
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia	
		December, 1988	

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

TABLE 1: Quantitative Solubility Studies of the Benzoic acid methyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Gilbert and Lauer (ref 1)	288-308	mutual	titration
Richon and Viallard (ref 2)	298	(1) in (2)	refractometric
Stephenson and Stuart (ref 3)	273-364	mutual	GLC

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. SOLUBILITY OF BENZOIC ACID METHYL ESTER (1) IN WATER (2)

All the available data for the solubility of benzoic acid methyl ester (1) in water (2) are summarized in Table 2 except that the approximate values of Gilbert and Lauer (ref 1) have been rejected because they are in general much higher than the other studies (ref 2,3).

At 298 K, the only temperature where comparison is possible, the data of Richon and Viallard (ref 2) and Stephenson and Stuart (ref 3) are in good agreement enabling the average value to be Recommended. At other temperatures only the data of Stephenson and Stuart (ref 3) are available and, pending further studies, they must be regarded as Tenative although it may be noted that the solubilities of these authors are usually reliable.

COMPONENTS:		EVALUATOR:
(1)	Benzoic acid methyl ester (methyl benzoate); C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[93-58-3]	Murdoch University, Perth, W.A.,
(2) Water: $H_{0}0$ : [7732)	Water: $H_0$ : $(7732-18-5)$	Australia
		December, 1988

# TABLE 2:Recommended (R) and Tentative Solubilitiesof Benzoic acid methyl ester (1) in Water (2)

T/K	Solubilities			
	Reported values	"Best" values <sup>2</sup>	ı	
	g(1)/100g sln	g(1)/100g sln	$10^{4}x_{1}$	
273	0.221 (ref 3)	0.22	2.9	
283	0.220 <sup>*</sup> (ref 3)	0.22	2.9	
293	0.223* (ref 3)	0.22	2.9	
298	0.202 (ref 2), 0.227 <sup>*</sup> (ref 3)	$0.215 \pm 0.013^{b}$ (R)	2.85 <sup>b</sup>	
303	0.233 <sup>*</sup> (ref 3)	0.23	3.0	
313	0.245 <sup>*</sup> ref 3)	0.25	3.3	
323	0.264 <sup>*</sup> (ref 3)	0.26	3.4	
333	0.287 <sup>*</sup> (ref 3)	0.29	3.8	
343	0.315 <sup>*</sup> (ref 3)	0.32	4.3	
353	0.347 <sup>*</sup> (ref 3)	0.35	4.7	
363	0.405 <sup>*</sup> (ref 3)	0.41	5.4	

a Rounded values of ref 3 except at 298 K.

<sup>b</sup> Average value; x<sub>1</sub> has the same status and (relative) percentage uncertainty as the mass % solubility.

# 2. SOLUBILITY OF WATER (2) IN BENZOIC ACID METHYL ESTER (1)

All the data for the solubility of water (2) in benzoic acid methyl ester (1) are summarized in Table 3. The two data sets (ref 1,3) are in fair agreement but in the absence of other independent studies the reported solubilities must be regarded as Tentative since the aqueous phase data of Gilbert and Lauer (ref 1) were rejected (see above). However, it may be noted that the data of Stephenson and Stuart (ref 3) are usually reliable.

COMPONENTS:	EVALUATOR:				
<ul> <li>(1) Benzoic acid methyl ester (methyl benzoate); C<sub>8</sub>H<sub>8</sub>O<sub>2</sub>; [93-58-3]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988				
CRITICAL EVALUATION: (continued)					
<u>TABLE 3: Tentat</u> of Water (2) in Benzoid	<u>ive Solubilities</u> c_acid_methyl_ester_(1)				
T/K Sol	ubilities				
Reported values	"Best" values <sup>a</sup>				
g(2)/100g sln	$g(2)/100g sln 10^2 x_2$				
273 0.46 (ref 3)	0.5 4				
283 0.54* (ref 3)	0.5 4				
293 0.4* (ref 1), 0.62* (ref 3)	0.6 5				
298 0.6 <sup>*</sup> (ref 1), 0.67 <sup>*</sup> (ref 3)	0.6 5				
303 0.9 <sup>*</sup> (ref 1), 0.73 <sup>*</sup> (ref 3)	0.7 5				
313 0.87 <sup>*</sup> (ref 3)	0.9 6				
323 1.02 (ref 3)	1.0 7				
333 1.18 <sup>*</sup> (ref 3)	1.2 9				
343 1.37 <sup>*</sup> (ref 3)	1.4 10				
353 1.60 <sup>*</sup> (ref 3)	1.6 11				
363 1.96 <sup>*</sup> (ref 3)	2.0 14				
<sup>a</sup> Rounded values of ref 3, see text.					
REFERENCES					
1. Gilbert, E. C.; Lauer, B. E. J.	Phys. Chem. <u>1927</u> , 31, 1050-2.				
2. Richon, D.; Viallard, A. Fluid Phase Equil. <u>1985</u> , 21, 279-93.					
3. Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.					

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COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Benzoic acid methyl ester (methyl benzoate); C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ;			Gilbert, E.C.; Lauer, B.E. J. Phys. Chem. <u>1927</u> , 31, 1050-2.		
[93	3-58-3]				
(2) Wat	cer; H <sub>2</sub> O; [7732-1	8-5]			
VARIABLES	3:		PREPARED BY:		
T/K = 28	38 - 308		A. Skrzecz		
EXPERIMEN	NTAL VALUES: Mutual solubility	of benzoic a	acid methyl ester and water		
t/°C	g(1)/10	0g sln	x1 (compiler)		
,	(2)-rich phase	(1)-rich phas	se (2)-rich phase (1)-rich phase		
15	0.1	99.8	0.00013 0.985		
25	0.4	99.4	0.00053 0.956		
35	0.5	98.8	0.00066 0.916		
		AUXILIARY	INFORMATION		
METHOD/AF	PARATUS/PROCEDUR	E:	SOURCE AND PURITY OF MATERIALS:		
The titration method was used as described by Walton and Jenkins (ref 1). A measured quantity of one component in a large test tube placed in a transparent constant temperature bath was titrated from a calibrated burette. The mixture was stirred rapidly with a motor stirrer and the equilibrium end point taken at the instant the solution became clear (with a lamp on the opposite side). The end points were sharp and easily dupli- cated. The temperature of the burette was recorded and from the density of the material the weight was computed. The solutions were			<ul> <li>(1) Eastman Kodak Company, chemically pure grade; redistilled under reduced pressure, a fraction boiling 88-91°C at 17mm Hg being collected.</li> <li>(2) Distilled.</li> </ul>		
			ESTIMATED ERROR:		
			Not specified.		
was computed. The solutions were carefully protected from moisture. The mutual solubility was determin- ed from the densities of the re- spective saturated solutions on the assumption that mixing laws were valid in the range of low concen- trations involved. Several runs were made at each temperature.		moisture. s determin- the re- ions on the aws were w concen- al runs ature.	REFERENCES: 1. Walton, J.H.; Jenkins, J.D. <i>J. Am. Chem. Soc.</i> <u>1923</u> , 45, 2555.		

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Benzoic acid methyl ester	Richon, D.; Viallard, A.	
(methyl benzoate); C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ; [93-58-3]	Fluid Phase Equilib. <u>1985</u> , 21, 279-93.	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of benzoic acid methyl ported to be 0.00149 mol(1)/100 g(2). mole fraction, $x_1$ , values calculated sln and 2.68 x 10 <sup>-4</sup> .	ester in water at 298.1 K was re- The corresponding mass per cent and by the compiler are 0.202 g(1)/100g	
AUXILIARY 1	INFORMATION	
METHOD/APPARATUS/PROCEDURE: The refractometric method was used. The Phoenix model 1-2000T differen- tial refractometer from Texas Instruments was used and the solu- bility was determined from a char- acteristic calibration curve as described in the thesis of Richon (ref 1).	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Source not specified; purified by preparation gas chromato- graphic method; purity &gt;99.5%, water content was negligible.</li> <li>(2) Distilled.</li> </ul>	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	
	1. Richon, D. <i>Thesis</i> , University de Clermont-Ferrand, <u>1974</u> .	

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COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Benzoic acid methyl ester			Stephenson, R.; S	Stuart, J.	
(methyl benzoate); C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ;		J. Chem. Eng. Data <u>1986</u> , 31,			
[93-58-	3]		56-70.		
(2) Water;	H <sub>2</sub> O; [7732-1	.8-5]			
VARIABLES:			PREPARED BY:		
T/K = 273 -	364		Z. Maczynska		
EXPERIMENTAL	VALUES:		L		
Mutua	l solubility	of benzoic a	cid methyl ester ar	nd water	
t/°C	q(1)/10	0g sln	x <sub>1</sub> (comp	viler)	
. (2)	-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase	
<u> </u>					
0	0.221	99.54	0.000293	0.9662	
9.7	0.221	99.46	0.000293	0.9606	
20.1	0.213	99.35	0.000282	0.9529	
29.6	0.282	99.27	0.000374	0.9473	
40.2	0.247	99.16	0.000327	0.9398	
49.8	0.258	99.02	0.000342	0.9304	
70.2	0.280	90.70 98.62	0.000379	0.9133	
80.3	0.358	98.44	0.000431	0.8930	
90.5	0.408	97.96	0.000542	0.8640	
std. dev.	0.002	0.02			
		AUXILIARY 1	INFORMATION		
METHOD/APPARA	TUS/PROCEDUR	E:	SOURCE AND PURITY	OF MATERIALS:	
The analytic	al method wa	s used.	(1) Source not sp	ecified. commer-	
Component (1	) was equili	brated	cial sample; purity 99%; used		
temperature	in a thermos	tat. Each	(2) Not specified.		
<pre>layer was sa: (1) was dete</pre>	mpled with a rmined by ad	syringe; ding a			
weighed amou	nt of aceton	itrile			
organic laye	s propanoi) r sample and	to the measuring			
by a Gow-Mac	thermal con	ductivity	ESTIMATED ERROR:		
(Chromosorb	101 packing	and a HP	Accuracy of method 0.1 wt% or less,		
3390 A record A similar pro	der-integrat ocedure but	or). a higher	for solubility, s	ee above.	
boiling mate	rial (e.g. 1	-hexanol)			
was used to water layer.	aetermine (2	) in the			
			References:		

COMPONENTS:	EVALUATOR:
<pre>(1) Benzoic acid, 2-hydroxy-, methyl ester (methyl salicylate); C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>; [119-36-8]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H <sub>2</sub> O; [7732-18-5]	March, 1990

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

#### <u>TABLE 1: Quantitative Solubility Studies of the</u> <u>2-Hydroxybenzoic acid methyl ester (1) - Water (2) System</u>

Reference	T/K	Solubility	Method
Seidell (ref 1)	288-303	(1) in (2)	titration
Stephenson and Stuart (ref 2)	273-364	mutual	GLC

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. SOLUBILITY OF 2-HYDROXYBENZOIC ACID METHYL ESTER (1) IN WATER (2)

All the available quantitative solubility data for the solubility of 2-hydroxybenzoic acid methyl ester (1) in water (2) are summarized in Table 2.

At 298 K the data of Seidell (ref 1) and Stephenson and Stuart (ref 2) are in excellent agreement. Furthermore Seidell reported the solubility of (1) in (2) was constant over the range 288-303 K which is consistent, within the limits of his likely experimental errors, with the more recent study of Stephenson and Stuart. This gives confidence in the reliability of the data of Stephenson and Stuart at other temperatures although, in the absence of confirmatory studies, their solubilities at temperatures other than 298 K must be regarded as Tentative.

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COMPONENTS:	EVALUATOR:
<pre>(1) Benzoic acid, 2-hydroxy-, methyl ester (methyl salicylate); C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>; [119-36-8]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H <sub>2</sub> O; [7732-18-5]	March, 1990

# TABLE 2: Recommended (R) and Tentative Solubilities of 2-Hydroxybenzoic acid methyl ester (1) in Water (2)

T/K	Solubi	ilities	
	Reported values	"Best" values	a
	g(1)/100g sln	g(1)/100g sln	10 <sup>4</sup> x <sub>1</sub>
273	0.12 <sup>*</sup> (ref 2)	0.12	1.4
283	0.12 <sup>*</sup> (ref 2)	0.12	1.4
293	0.12 <sup>*</sup> (ref 2)	0.12	1.4
298	0.12 (ref 1), 0.12 <sup>*</sup> (ref 2)	0.12 (R)	1.4
303	0.13 (ref 2)	0.13	1.5
313	0.15 (ref 2)	0.15	1.8
323	0.17 <sup>*</sup> (ref 2)	0.17	2.0
333	0.20 <sup>*</sup> (ref 2)	0.20	2.4
343	0.22 <sup>*</sup> (ref 2)	0.22	2.6
353	0.25 <sup>*</sup> (ref 2)	0.25	2.9
363	0.27 <sup>*</sup> (ref 2)	0.27	3.2

a Values of ref 2, see text.

2. SOLUBILITY OF WATER (2) IN 2-HYDROXYBENZOIC ACID METHYL ESTER (1)

The only data available for the solubility of water (2) in 2hydroxybenzoic acid methyl ester (1) are those of Stephenson and Stuart (ref 2) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the original solubility values but it may be noted that the data of these authors are usually reliable.

# REFERENCES

1.	Seidell,	Α.	Hygienic	Lab.	Bull.	<u>1910,</u>	No.	67,	98pp.	(U.S.	Govt.
	Printing	Off:	ice, Washi	ingto	n, DC)	•					

2. Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u>, 31, 56-70.

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<pre>COMPONENTS: (1) Benzoic acid, 2-hydroxy-, methyl ester (methyl salicylate); C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>; [119-36-8] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Seidell, A. <i>Hygienic Lab. Bull.</i> <u>1910</u> , No. 67, 98 pp (US Govt. Printing Office, Washington, DC).
VARIABLES: T/K = 288 - 303	PREPARED BY: G.T. Hefter
EXPERIMENTAL VALUES: The solubility of 2-hydroxybenzoic ac reported to be 0.12 g(1)/100g sln. Th value calculated by the compiler is 1 The solubility of 2-hydroxybenzoic ac (15-30°C) was reported to be constant 0.1 cm <sup>3</sup> (1)/100cm <sup>3</sup> (2).	bid methyl ester in water at 25°C was ne corresponding mole fraction, $x_1$ , 1.4 x 10 <sup>-4</sup> . Did methyl ester at other temperatures t with an approximate value of
AUXILIARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE: The titration method was used. Por- tions (50 cm <sup>3</sup> ) of (2) were placed in an Erlenmeyer flask and titrated with (1) to opalescence. The flask and its contents were then cooled to the lowest temperature desired and allowed to warm slowly. The temperature was continuously re- corded with a thermometer and the last drop or two of (1) was added as the desired temperature was reached.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not stated; purified by fractional distillation; b.p. 220-221°C, d25 1.182 g/cm3. (2) Distilled (no details given).  ESTIMATED ERROR: Temp. not stated. Soly. not stated. REFERENCES: </pre>

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COMPONENTS:			ORI	GINAL MEASUREME	NTS:	
(1) Benzo	ic acid, 2-hyd	roxy-,	st	ephenson, R.; S	tuart, J.	
methy	l ester		J. Chem. Eng. Data <u>1986</u> , 31,			
(meth	yi salicylate)	; C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> ;		56-70.		
[119-	30-0]					
(2) Water	; H <sub>2</sub> O; [7732-1	8-5]				
VARIABLES:			PRE	PARED BY:		
T/K = 273	- 364		Z.	Maczynska		
EXPERIMENTA	L VALUES:				**************************************	
Mutual	solubility of	2-hydroxybenz	zoic	acid methyl est	er and water	
				······································	• •	
t/°C	g(1)/10	Dg sln		$x_1$ (comp	iler)	
(	2)-rich phase	(1)-rich phas	se 	(2)-rich phase	(1)-rich phase	
0	0.116	99.84		0.000137	0.9866	
9.5	0.131	99.83		0.000155	0.9858	
19.9	0.120	99.74		0.000142	0.9784	
29.7	0.124	99.70		0.000147	0.9752	
39.5	0.145	99.66		0.000172	0.9720	
50.0	0.175	99.59		0.000207	0.9664	
60.1	-	99.52		-	0.9608	
70.2	0.221	99.40		0.000262	0.9515	
80.1	0.270	99.25		0.000320	0.9400	
90.5	0.270	99.20		0.000320	0.9362	
std. dev	. 0.004	0.01				
		AUXILIARY :	INFO	RMATION		
			COT		OF MAREPTATC.	
METHOD/APPA	RATUS/PROCEDUR.	L ;	500	RCE AND PURITY	OF MATERIALS:	
The analyt	ical method was	s used. brated	(1) Source not specified, commer-			
with composite	nent (2) at a	given		as received.	puricy 99%, used	
temperatur	e in a thermost sampled with a	tat. Each	1 12	) Not specified		
(1) was de	termined by add	ding a		, not specified	•	
<pre>weighed am  (or sometic</pre>	ount of aceton: mes propanol)	itrile to the				
organic la	yer sample and	measuring	FCu	TMATED EDDOD.		
by a Gow-M gc the (1)	ac thermal cond /acetonitrile	ductivity peak ratio	101	IMALED EKKUK;		
(Chromosor	b 101 packing	and a HP	Ac	curacy of metho	d 0.1 wt% or less,	
A similar	order-integrate procedure but a	or). A higher		- BOLUNITICA' B		
boiling ma	terial (e.g. 1	-hexanol)				
was used to water lave	o determine (2) r.	in the		FDENCES.		
			REF	ERENCES:		

COMPC	DNENTS:	EVALUATOR:
(1)	Acetic acid cyclohexyl ester ( <i>cyclohexyl acetate</i> ); C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> ; [622-45-7]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988

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

TABLE 1: Quantitative Solubility Studies of the Acetic acid cyclohexyl ester (1) - Water (2) System

		A STATUTE OF A STATU	the second s
Reference	T/K	Solubility	Method
Doolittle (ref 1)	293	mutual	unspecified
Othmer et al. (ref 2)	297	mutual	unspecified
Stephenson and Stuart (ref 3)	273-363	mutual	GLC

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. SOLUBILITY OF ACETIC ACID CYCLOHEXYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid cyclohexyl ester (1) in water (2) are summarized in Table 2 with the exception of the datum of Doolittle (ref 1) which is substantially lower than other data (ref 2,3) and has therefore been rejected.

At 296.7 K, the only temperature where comparison is possible, the data of Othmer et al. (ref 2) and Stephenson and Stuart (ref 3) are in good agreement and the average value is Recommended. At other temperatures only the data of Stephenson and Stuart (ref 3) are available and, pending further studies, must be regarded as Tentative, although it may be noted that solubilities reported by these authors are usually reliable.

COMPO	DNENTS:	EVALUATOR:
(1)	Acetic acid cyclohexyl ester ( <i>cyclohexyl acetate</i> ); C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> ; [622-45-7]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988

TABLE 2:	Recommended	(R) an	<u>d_Tentat</u> :	ive_Solul	bilities
of Acet	ic acid cyclo	hexyl e	ester (1)	in Wate	r (2)

Solubilities		
Reported values	"Best" values é	1
g(1)/100g sln	g(1)/100g sln	10 <sup>4</sup> x <sub>1</sub>
0.393 (ref 3)	0.39	5.0
0.325 <sup>*</sup> (ref 3)	0.33	4.2
0.292 <sup>*</sup> (ref 3)	0.29	3.7
0.29 (ref 2), 0.282 <sup>*</sup> (ref 3)	0.286 ± 0.006 (R) <sup>b</sup>	3.63 <sup>b</sup>
0.277 <sup>*</sup> (ref 3)	0.28	3.6
0.264 <sup>*</sup> (ref 3)	0.26	3.3
0.242 <sup>*</sup> (ref 3)	0.24	3.0
0.225 <sup>*</sup> (ref 3)	0.23	2.9
0.217 <sup>*</sup> (ref 3)	0.22	2.8
0.224 <sup>*</sup> (ref 3)	0.22	2.8
0.247 <sup>*</sup> (ref 3)	0.25	3.2
0.290 <sup>*</sup> (ref 3)	0.29	3.7
	Solubilit Reported values g(1)/100g sln 0.393 (ref 3) 0.325* (ref 3) 0.292* (ref 3) 0.292* (ref 3) 0.277* (ref 3) 0.264* (ref 3) 0.264* (ref 3) 0.225* (ref 3) 0.217* (ref 3) 0.224* (ref 3) 0.224* (ref 3) 0.224* (ref 3) 0.224* (ref 3)	Solubilities         "Best" values           g(1)/100g sln         g(1)/100g sln         g(1)/100g sln           0.393 (ref 3)         0.39         0.33           0.292* (ref 3)         0.29         0.29           0.291 (ref 2), 0.282* (ref 3)         0.286 ± 0.006 (R) <sup>b</sup> 0           0.277* (ref 3)         0.286 ± 0.006 (R) <sup>b</sup> 0           0.264* (ref 3)         0.286         0.26           0.225* (ref 3)         0.28         0.24           0.225* (ref 3)         0.24         0.24           0.217* (ref 3)         0.22         0.23           0.217* (ref 3)         0.22         0.24           0.224* (ref 3)         0.22         0.24           0.224* (ref 3)         0.25         0.25           0.247* (ref 3)         0.25         0.25

<sup>a</sup> Rounded values of ref 3 except at 296.7 K.

<sup>b</sup> Average value; x<sub>1</sub> has the same status and (relative) percentage uncertainty as the mass % solubility.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID CYCLOHEXYL ESTER (1)

All the available solubility data for water (2) in acetic acid cyclohexyl ester (1) are summarized in Table 3. Serious disagreement exists between the values reported (at slightly different temperatures) by Doolittle (ref 1) and Othmer et al. (ref 2) on the one hand and Stephenson and Stuart (ref 3) on the other. In the absence of confirmatory studies it is not possible to distinguish between these data and thus no Critical Evaluation is possible, although it may be noted that the data of Stephenson and Stuart (ref 3) are usually reliable.

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COMPONENTS:	EVALUATOR:
<ul> <li>(1) Acetic acid cyclohexyl ester (cyclohexyl acetate); C<sub>8</sub>H<sub>14</sub>O<sub>2</sub>; [622-45-7]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988
CRITICAL EVALUATION: (continued)	<u> </u>
<u>TABLE 3: Repor</u> of Water (2) in Acetic a	ted Solubilities acid cyclohexyl ester (1)
T/K Sol	lubilities
Reported values	"Best" values <sup>a</sup>
g(2)/100g sln	$10^2 x_2^{a}$
273 0.67 (ref 3)	5.1
283 0.65 <sup>*</sup> (ref 3)	5.0
293 1.42 (ref 1), 0.70 <sup>*</sup> (ref 3)	5.3
298 1.45 <sup>b</sup> (ref 2), 0.74 <sup>*</sup> (ref 3	) 5.6
303 0.80 <sup>*</sup> (ref 3)	6.0
313 0.91 <sup>*</sup> (ref 3)	6.8
323 1.00 <sup>*</sup> (ref 3)	7.4
333 1.05 <sup>*</sup> (ref 3)	7.7
343 1.07* (ref 3)	7.9
353 1.15 <sup>*</sup> (ref 3)	8.4
363 1.36 <sup>*</sup> (ref 3)	9.8
<sup>a</sup> Rounded values of ref 3, see text.	
<sup>ь</sup> 296.7 К.	
REFERENCES	
1. Doolittle, A. K. Ind. Eng. Chem.	. <u>1935</u> , 27, 1169-79.
<ol> <li>Othmer, D. F.; White, R. E.; Tr 1240-8; ibid. 1513.</li> </ol>	ueger, E. Ind. Eng. Chem. <u>1941</u> , 33,
3. Stephenson, R.; Stuart, J. J. C	hem. Eng. Data <u>1986</u> , 31, 56-70.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid cyclohexyl ester	Doolittle, A.K.
(cyclohexyl acetate); C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> ; [622-45 <b>-</b> 7]	Ind. End. Chem. <u>1935</u> , 27, 1169-79.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of acetic acid cyclohe ported to be 0.16 g(1)/100g sln. The value calculated by the compiler is 2 The solubility of water in acetic aci ported to be 1.42 g(2)/100g sln. The value calculated by the compiler is 0	exyl ester in water at 20°C was re- corresponding mole fraction, $x_1$ , 2.0 x 10 <sup>-4</sup> . d cyclohexyl ester at 20°C was re- corresponding mole fraction, $x_2$ , 0.102.
AUXILIARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commer- cial product; purity 79%, b.p. range 165-193°C, $d_4^{20}$ 0.963. (2) Not specified.
	(-,
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid cyclohexyl ester (cyclohexyl acetate); C<sub>8</sub>H<sub>14</sub>O<sub>2</sub>;</pre>	Othmer, D.F.; White, R.E.; Trueger, E.
[622-45-7]	Ind. Eng. Chem. <u>1941</u> , 33, 1240-8, 1513.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 297	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of acetic acid cycloho ported to be 0.29 g(1)/100g sln. The value calculated by the compiler is : The solubility of water in acetic ac: ported to be 1.45 g(2)/100g sln. The value calculated by the compiler is (	exyl ester in water at 23.5°C was re- corresponding mole fraction, $x_1$ , 3.7 x 10 <sup>-4</sup> . id cyclohexyl ester at 23.5°C was re- corresponding mole fraction, $x_2$ , 0.104.
AUXILIARY	INFORMATION
	SOUDOF AND DUDTHY OF MAMEDIALS.
Nothing was aposified in the paren	(1) Not specified
Mouning was specified in the paper.	(1) Not specified
	(2) Not specified.
	ESTIMATED ERROR:
	Temp. ±0.5 <sup>o</sup> C (mean of reported range).
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:			
<ol> <li>Acetic acid cyclohexyl ester</li> </ol>	Stephenson, R.; Stuart, J.			
(cyclohexyl acetate); C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> ;	J. Chem. Eng. Data <u>1986</u> , 31,			
[622-45-7]	56-70.			
(2) Water; H <sub>2</sub> O; [7732-18-5]				
VARIABLES:	PREPARED BY:			
T/K = 273 - 363	Z. Maczynska			
EXPERIMENTAL VALUES:				
Mutual solubility of acetic aci	d cyclohexyl ester and water			
t/°C g(1)/100g sln	x <sub>1</sub> (compiler)			
(2)-rich phase (1)-rich phas	e (2)-rich phase (1)-rich phase			
0 0.393 99.33	0.000499 0.9494			
9.4 0.317 99.35	0.000403 0.9509			
19.8 0.304 99.29	0.000386 0.9466			
29.7 0.260 99.21	0.000330 0.9408			
39.6 0.251 99.10	0.000319 0.9331			
49.8 0.229 99.01	0.000291 0.9268			
60.1 0.218 98.95	0.000277 0.9227			
70.0 0.224 98.93	0.000284 0.9213			
80.1 0.257 98.85	0.000326 0.9159			
90.3 0.286 98.64	0.000363 0.9018			
std. dev. 0.002 0.01				
	.NFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The analytical method was used.	(1) Source not specified, commer-			
Component (1) was equilibrated	cial sample; purity 99%; used			
temperature in a thermostat. Each				
layer was sampled with a syringe;	(2) Not specified.			
weighed amount of acetonitrile				
(or sometimes propanol) to the				
by a Gow-Mac thermal conductivity	ESTIMATED ERROR:			
gc the (1)/acetonitrile peak ratio	Accuracy of method 0.1 wt% or less.			
3390 A recorder-integrator).	for solubility, see above.			
A similar procedure but a higher				
was used to determine (2) in the				
water layer.	REFERENCES:			

СОМРО	NENTS:	EVALUATOR:
(1)	Butanedioic acid diethyl ester ( <i>diethyl succinate</i> ); C <sub>8</sub> H <sub>14</sub> O <sub>4</sub> ; [123-25-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988

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

TABLE 1: Quantitative Solubility Studies of the Butanedioic acid diethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Sobotka and Kahn (ref 1)	293	(1) in (2)	titration
Stephenson and Stuart (ref 2)	274-364	mutual	GLC

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. SOLUBILITY OF BUTANEDIOIC ACID DIETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of butanedioic acid diethyl ester (1) in water (2) are summarized in Table 2. At 293 K, the only temperature where comparison is possible, the data of Sobotka and Kahn (ref 1) and Stephenson and Stuart (ref 2) are in good agreement and the average value is Recommended. At other temperatures only the data of Stephenson and Stuart (ref 2) are available and must therefore be regarded as Tentative although it may be noted that the solubilities reported by these authors are generally reliable.

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COMPONENTS:	EVALUATOR:		
<ul> <li>(1) Butanedioic acid diethyl ester (<i>diethyl succinate</i>); C<sub>8</sub>H<sub>14</sub>O<sub>4</sub>; [123-25-1]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988		
CRITICAL EVALUATION: (continued)			
<u>TABLE 2: Recommended (R)</u> of Butanedioic acid dieth	<u>and Tentative Solubilities</u> yl ester (1) in Water (2)		
T/K Sol	ubilities		
Reported values	"Best" values <sup>a</sup>		
g(1)/100g sln	$g(1)/100g \ sln \ 10^3 x_1$		
273 2.86 (ref 2)	2.9 3.0		
283 2.50 <sup>*</sup> (ref 2)	2.5 2.6		
293 1.89 (ref 1), 2.17 <sup>*</sup> (ref 2)	$2.03 \pm 0.14 (R)^{b}$ $2.14^{b}$		
298 2.15* (ref 2)	2.2 2.3		
303 1.95* (ref 2)	2.0 2.1		
313 1.81* (ref 2)	1.8 1.9		
323 1.75 <sup>*</sup> (ref 2)	1.8 1.9		
333 1.75* (ref 2)	1.8 1.9		
343 1.78* (ref 2)	1.8 1.9		
353 1.86* (ref 2)	1.9 2.0		
363 2.05* (ref 2)	2.1 2.2		

<sup>a</sup> Rounded values of ref 2 except at 293 K.

<sup>b</sup> Average value;  $x_1$  has the same status and (relative) percentage uncertainty as the mass % solubility.

2. SOLUBILITY OF WATER (2) IN BUTANEDIOIC ACID DIETHYL ESTER (1)

The only data available for the solubility of water (2) in butanedioic acid diethyl ester (1) are those of Stephenson and Stuart (ref 2) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental solubilities but it may be noted that the data of these authors are usually reliable.

REFERENCES

1.	Sobotka,	н.;	Kahn,	J.	J.	Am.	Chem.	Soc.	<u>1931</u> ,	53, 2	2935-8	3.
2.	Stephenso	n, R	.; st	uart,	ј.	J.	Chem.	Eng.	Data	<u>1986</u>	, 31,	56-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butanedioic acid diethyl ester	Sobotka, H.; Kahn, J.
( <i>diethyl succinate</i> ); C <sub>8</sub> H <sub>14</sub> O <sub>4</sub> ;	<i>J. Am. Chem. Soc.</i> <u>1931</u> , 53,
[123-25-1]	2935-8.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanedioic acid diethyl ester in water at  $20^{\circ}$ C was reported to be 1.92 g(1)/100mL(2). The corresponding mass per cent and mole fraction,  $x_1$ , values calculated by the compiler are 1.89 g(1)/100g sln and 0.00199.

Density of water  $d_4^{20} = 0.9982$  (ref 1) was used in the calculation.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The titration method was used. The ester was added dropwise from a	SOURCE AND PURITY OF MATERIALS: (1) Source not specified (Eastman Kodak Laboratories or synthe-
micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The	sized); twice-distilled under reduced pressure; $d_4^{20}$ 1.0402, $n_D^{20}$ 1.4200.
bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV	(2) Distilled.
dye was put into the water to im- prove the end-point of the titra- tion at actuation one additional	ESTIMATED ERROR:
drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent droplets.	Not specified.
-	REFERENCES:
	<ol> <li>Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, <u>1973</u>.</li> </ol>

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COMPONENTS:			ORIGINAL MEASUREMENTS:	
(1) Butanedioic acid diethyl ester			Stephenson, R.; Stuart, J.	
(diethyl succinate); C <sub>8</sub> H <sub>14</sub> O <sub>4</sub> ; [123-25-1]			J. Chem. Eng. Data <u>1986</u> , 31, 56-70.	
(2) Water; H <sub>2</sub> O; [7732-18-5]				
VARIABLES:			PREPARED BY:	
T/K = 273 - 364			Z. Maczynska	
EXPERIMENTAL VALUES:				
Mutual solubility of butanedioic acid diethyl ester and water				
$t/^{\circ}C$ g(1)/100g sln			x <sub>1</sub> (compiler)	
(2)-rich phase (1)-rich phase			e (2)-rich phase	(1)-rich phase
0	2.86	98.72	0.00303	0.8886
10.0	2.67	98.49	0.00283	0.8709
20.0	2.13	98.22	0.00225	0.8509
29.7	1.99	97.92	0.00209	0.8296
39.8	1.79	97.58	0.00188	0.8066
50.0	1,79	97.13	0.00188	0.7778
60.3	1.74	96.76	0.00183	0.7554
70.0	1.79	96.40	0.00188	0.7347
80.1	1.84	96.03	0.00193	0.7144
90.7	2.09	95.77	0.00220	0.7007
std. dev. 0.05 0.07				
AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.			SOURCE AND PURITY OF MATERIALS:	
			(1) Source not specified, commer- cial sample; purity 99%; used as received.	
			(2) Not specified.	
			,	
			ESTIMATED ERROR:	
			Accuracy of method 0.1 wt% or less, for solubility, see above.	
			REFERENCES:	
COMPONEN	TS:	ORIGINAL MEASUREMENTS:		
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(1) 2, (2	3-Butanediol diacetate ,3-butylene diacetate);	Othmer, D.F.; Bergen, W.S.; Shlechter, N.; Bruins, P.F.		
C <sub>8</sub>	H <sub>14</sub> O <sub>4</sub> ; [1114-92-7]	Ind. Eng. Chem. <u>1945</u> , 37, 890-4.		
(2) Wa	ter; H <sub>2</sub> O; [7732-18-5]			
VARIABLE	S:	PREPARED BY:		
T/K = 2	99 - 348	A. Skrzecz		
EXPERIME	NTAL VALUES: Mutual solubility of 2,3-But	anediol diacetate and water		
+ 1%	a(1)/100a sln	x. (compiler)		
τ, τ	(2)-rich phase (1)-rich pha	se (2)-rich phase (1)-rich phase		
26	3.62 96.3	0.00387 0.729		
50	2.87 96.6	0.00305 0.746		
75	3.7 95.9	0.00396 0.708		
	AUXILIARY	INFORMATION		
METHOD/AI	PPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Presumal ported 1	bly the titration method re- by Othmer, White and Trueger	(1) Synthesized from meso-2,3-buty- lene glycol; b.p. range 1°C.		
(ref 1) ported t system 2 water-2 diacetat	Was used. The data were re- together with the ternary 2,3-Butanediol diacetate- ,3-butanediol (2,3-butylene te-water-butylene glycol).	(2) Not specified.		
		ESTIMATED ERROR:		
		Not specified.		
		REFERENCES:		
		1. Othmer, D.F.; White, R.E.; Trueger,E. Ind. Eng. Chem. <u>1941</u> , 33, 1240.		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Hexanedioic acid dimethyl	Stephenson, R.; Stuart, J.		
ester (dimethyl adipate);	J. Chem. Eng. Data <u>1986</u> , 31,		
$C_{8}H_{14}O_{4}; [627-93-0]$	56-70.		
(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 282 - 364	Z. Maczynska		
EXPERIMENTAL VALUES:			
Mutual solubility of hexanedioid	c acid dimethyl ester and water		
$t/^{\circ}C$ $q(1)/100q sln$	X1 (Compiler)		
(2)-rich phase (1)-rich phas	se (2)-rich phase (1)-rich phase		
9.2 3.81 98.06	0.00408 0.8394		
19.6 3.07 97.70	0.00326 0.8146		
30.9 2.85 97.33	0.00302 0.7903		
39.5 2.77 96.93	0.00294 0.7655		
49.8 2.70 96.34	0.00286 0.7313		
60.0 2.73 95.90	0.00289 0.7075		
70.5 2.87 95.27	0.00305 0.6756		
80.2 3.50 94.59	0.00374 0.6439		
90.5 3.23 94.28	0.00344 0.6302		
std. dev. 0.06 0.06			
AUXILIARY :	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The analytical method was used.	(1) Source not specified, commer-		
Component (1) was equilibrated	cial sample; purity 98%; used		
temperature in a thermostat. Each	as receiveu.		
layer was sampled with a syringe;	(2) Not specified.		
weighed amount of acetonitrile			
(or sometimes propanol) to the organic layer sample and measuring			
by a Gow-Mac thermal conductivity	ESTIMATED ERROR:		
(Chromosorb 101 packing and a HP	Accuracy of method 0.1 wt% or less,		
3390 A recorder-integrator). A similar procedure but a higher	for solubility, see above.		
boiling material (e.g. 1-hexanol)			
was used to determine (2) in the water layer.	DEFEDENCES.		
-	REFERENCED:		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 1,3-dimethylbutyl	Doolittle, A.K.
ester (1,3-dimethylbutyl	Ind. End. Chem. <u>1935</u> , 27, 1169-79.
$acecace; C_8H_{16}O_2; [108-84-9]$	
(2) water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES:	J
The solubility of acetic acid 1,3-dir	methylbutyl ester in water at 20 <sup>0</sup> C was
reported to be 0.08 g(1)/100g sln. The	ne corresponding mole fraction, $x_1$ ,
value calculated by the compiler is 1	$1.0 \times 10^{-4}$ .
The solubility of water in acetic aci	id 1.3-dimethylbutyl ester at $20^{\circ}$ C was
reported to be 0.89 g(2)/100g sln. Th	The corresponding mole fraction, $x_2$ ,
value calculated by the compiler is (	.067.
-	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commer-
	cial product; purity 95%, b.p. range 140-147°C, $d_4^{20}$ 0.857,
	$n_{\rm D}^{20}$ 1.4008.
	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Acetic acid 2-ethyl-1-butyl	Doolittle, A.K.		
ester (2-ethylbutyl acetate);	Ind End Chem 1935 27 1169-79		
C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [10031-87-5]	1114. End. Chem. <u>1955</u> , 27, 1109-79.		
(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 293	A. Skrzecz		
The solubility of acetic acid 2-ethyl	-1-butyl ester in water at 20°C was		
reported to be $0.06 \text{ g(1)}/100\text{g sln. Th}$	The corresponding mole fraction, $x_1$ ,		
value calculated by the compiler is 7	7 x 10 <sup>-5</sup> .		
The solubility of water in acetic aci	d 2-ethyl-1-butyl ester at 20°C was		
reported to be 0.75 g(2)/100g sln. The value calculated by the compiler is f	the corresponding mole fraction, $x_2$ ,		
Value calculated by the compiler is t			
AUXILIARY 1	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The method was not specified.	(1) Source not specified, commer- cial product; purity 91%, b.p. range 157-164°C, $d_4^{20}$ 0.876, $n_0^{20}$ 1.4103.		
	(2) Not specified.		
	-		
	ESTIMATED ERROR:		
	Not specified.		
	-		
	DEEDENOEG		
	REFERENCES:		

COMPONENTS:	EVALUATOR:
(1) Acetic acid hexyl ester (hexyl acetate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,
[142-92-7]	Murdoch University, Perth, W.A.,
(2) Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988

CRITICAL EVALUATION:

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

TABLE_	1:	Qua	ntita	<u>tive</u>	Solu	<u>bil</u> :	ity	Stu	<u>dies</u>	of	the
Aceti	. <u>c</u> _a	acid	hexyl	este	er (1)	)	Wat	er	(2)	Syst	:em

	······································		
Reference	T/K	Solubility	Method
Massaldi and King (ref 1)	298	(1) in (2)	GLC
Alvarez and Neila (ref 2)	298	mutual	titration
Stephenson and Stuart (ref 3)	273-363	mutual	GLC

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. SOLUBILITY OF ACETIC ACID HEXYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid hexyl ester (1) in water (2) are summarized in Table 2 with the exception of the approximate value of Alvarez and Neila (ref 2) which is much higher than the other studies (ref 1,3) and is therefore rejected. At 298 K, the only temperature where comparison is possible, the data of Massaldi and King (ref 1) and Stephenson and Stuart (ref 3) are in excellent agreement and the average value is Recommended. At other temperatures only the values of Stephenson and Stuart (ref 3) are available. Although their results for this system are rather scattered, the solubilities reported by these authors are generally reliable and pending further studies can be considered as Tentative.

100						
COMPONENTS:		EVALUATOR:				
(1) Acetic acid hexyl ester ( <i>hexyl acetate</i> ); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [142-92-7]		G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,				
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988				
CRITI	CRITICAL EVALUATION: (continued)					
	<u>TABLE 2: Recommended (R)</u> of Acetic acid hexyl	<u>and Tentative Solubilitie</u> ester (1) in Water (2)	25			
Т/К	So	lubilities				
	Reported values	"Best" value	s <sup>a</sup>			
	g(1)/100g sln	g(1)/100g sln	10 <sup>5</sup> x <sub>1</sub>			
273	0.084 (ref 3)	0.08	10			
283	0.066 (ref 3)	0.07	9			
293	0.056 <sup>*</sup> (ref 3)	0.06	7			

 $0.052 \pm 0.001 (R)^{b}$ 

0.05

0.05

0.05

0.05

0.06

0.06

6.5

6

6

6

6

7

7

9

363	0.066*	(ref 3)	0.07

0.051 (ref 1), 0.053 (ref 3)

0.052\* (ref 3)

0.051\* (ref 3)

0.051<sup>\*</sup> (ref 3)

0.052\* (ref 3)

0.056<sup>\*</sup> (ref 3)

 $0.060^*$  (ref 3)

298

303

313

323

333

343

353

a Rounded values of ref 3 except at 298 K.

<sup>b</sup> Average value;  $x_1$  has same status and (relative) percentage uncertainty as the mass % solubility.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID HEXYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid hexyl ester (1) are listed in Table 3. At 298 K, the only temperature where comparison is possible, the approximate value of Alvarez and Neila (ref 2) is not in very good agreement with the interpolated datum of Stephenson and Stuart (ref 3). Consequently, in the absence of other independent studies, all the data must be regarded as very Tentative. However, it may be noted that the solubilities reported by Stephenson and Stuart (ref 3) are generally reliable although the present values are rather scattered.

COMPONENTS:	EVALUATOR:		
<ol> <li>Acetic acid hexyl ester (hexyl acetate); C<sub>8</sub>H<sub>16</sub>O<sub>2</sub>;</li> </ol>	G.T. Hefter, School of Mathematical and Physical Sciences,		
[142-92-7]	Murdoch University, Perth, W.A.,		
(2) Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988		

CRITICAL EVALUATION: (continued)

# TABLE 3: Tentative Solubilities of Water (2) in Acetic acid hexyl ester (1)

T/K	Solubilities					
	Reported values	"Best" values <sup>a</sup>				
	g(2)/100g sln	g(2)/100g sln	$10^2 x_2$			
273	0.494 (ref 3)	0.5	4			
283	0.54 <sup>*</sup> (ref 3)	0.5	4			
293	0.58 <sup>*</sup> (ref 3)	0.6	5			
298	1.1 <sup>b</sup> (ref 2), 0.61 <sup>*</sup> (ref 3)	0.6	5			
303	0.63 <sup>*</sup> (ref 3)	0.6	5			
313	0.66 <sup>*</sup> (ref 3)	0.7	5			
323	0.69 <sup>*</sup> (ref 3)	0.7	5			
333	0.72 <sup>*</sup> (ref 3)	0.7	5			
343	0.74 <sup>*</sup> (ref 3)	0.7	5			
353	0.76 <sup>*</sup> (ref 3)	0.8	6			
363	0.78 <sup>*</sup> (ref 3)	0.8	6			

<sup>a</sup> Rounded values of ref 3, see text.

<sup>b</sup> Not included in "Best" value.

REFERENCES

1. Massaldi, H. A.; King, C. J. J. Chem. Eng. Data 1973, 18, 393-7.

2. Alvarez, J. R.; Neila, J. J. An. Quim. <u>1978</u>, 74, 326-32.

3. Stephenson, R.; Stuart, J. J. Chem. Eng. Data 1986, 31, 56-70.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid hexyl ester	Massaldi, H.A.; King, C.J.
(hexyl acetate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [142-92-7]	J. Chem. Eng. Data <u>1973</u> , 18, 393-7.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	Z. Maczynska
The solubility of acetic acid hexyl be 0.00354 mol(1)/L sln.	ester in water at 25°C was reported to
AUXILIARY	INFORMATION
	COURCE AND DUDIEV OF MAREDIALC.

The analytical method was used. A technique based on head-space analysis using gas-liquid chromatography was developed to determine solubilities of sparingly soluble organics. Saturated solutions need not be prepared in advance; thus, phase separation problems were avoided. Furthermore, the analysis of liquid samples was not required. This method is versatile enough to give determinations provided that the vapor pressure of the pure liquid substance is known. The gas chromatograph was a Varian Aerograph Model 1740 with a flame ionization detector.  Eastman Kodak Co., reagent grade; purity not specified; used as received.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.05°C.

**REFERENCES:** 

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid hexyl ester	Alvarez, J.R.; Neila, J.J.	
(hexyl acetate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [142-92-7]	An. Quim. <u>1978</u> , 74, 326-32.	
(2) water; $H_20$ ; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	Z. Maczynska .	
EXPERIMENTAL VALUES: The solubility of acetic acid hexyl ester in water at 25°C was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calculat- ed by the compiler is 0.00013.		
The solubility of water in acetic acid hexyl ester at $25^{\circ}$ C was reported to be 1.1 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calculat-		

ed by the compiler is 0.082.

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AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: Presumably the titration method was used. The data were reported to- gether with the ternary system acetic acid hexyl ester-water- phenol. No further details were reported in the paper.	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Source not specified, commercial product; used as received; d<sub>4</sub><sup>21.3</sup> 0.8681, n<sub>D</sub><sup>20</sup> 1.4093.</li> <li>(2) Twice distilled over KMnO<sub>4</sub>.</li> </ul>		
	Not specified. REFERENCES:		

COMPONENT	'S:		ORIGINAL MEASUREME	NTS:
(1) Acetic acid hexyl ester		Stephenson, R.; Stuart, J.		
(hexyl acetate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [142-92-7]		J. Chem. Eng. Data <u>1986</u> , 31, 56-70.		
(2) Wat	er; H <sub>2</sub> O; [7732-1	8-5]		
VARIABLES	:		PREPARED BY:	
T/K = 27	3 - 363		Z. Maczynska	
EXPERIMEN	TAL VALUES:			
	Mutual solubilit	y of acetic a	acid hexyl ester and	water
t/°C	g(1)/10	0g sln	x <sub>1</sub> (comp	iler)
	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase
0	0.084	99.506	0.000105	0.96177
9.5	0.070	99.504	0.000087	0.96162
19.7	0.043	99.434	0.000054	0.95641
29.6	0.054	99.270	0.000067	0.94441
40.0	0.056	99.254	0.000070	0.94325
50.0	0.047	99.367	0.000059	0.95148
60.7	0.051	99.305	0.000064	0.94695
70.0	0.057	99.251	0.000071	0.94303
80.0	0.063	99.220	0.000079	0.94079
90.2	0.066	99.215	0.000082	0.94044
std. d	ev. 0.003	0.004		
		AUXILIARY :	INFORMATION	
METHOD/AP	PARATUS/PROCEDUR	E:	SOURCE AND PURITY	OF MATERIALS:
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol)		(1) Source not sp cial sample; j as received.	ecified, commer- purity 99%; used	
		(2) Not specified		
		ESTIMATED ERROR:		
		Accuracy of method for solubility, se	d 0.1 wt% or less, ee above.	
was used water lay	yer.	, in the	REFERENCES:	

COMPO	DNENTS:	EVALUATOR:
(1)	Acetic acid 1-methylpentyl ester (1-methylpentyl	G.T. Hefter, School of Mathematical and Physical Sciences,
	acetate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [5953-49-1]	Murdoch University, Perth, W.A.,
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988

CRITICAL EVALUATION:

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

TABLE 1: Quantitative Solubility Studies of the Acetic acid 1-methylpentyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Park and Hopkins (ref 1)	298	(1) in (2)	unspecified
Doolittle (ref 2)	293	mutual	unspecified

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

Unfortunately, the data for the solubility of acetic acid 1-methylpentyl ester (1) in water (2) in both the publications listed in Table 1 are only semiquantitative. According to Park and Hopkins (ref 1) the solubility of (1) in (2) is less than 0.14 g(1)/100 g sln. Doolittle (ref 2) merely indicates (1) is "very slightly soluble" in (2).

For the solubility of water (2) in 1-methylpentyl acetate (1) only the datum of Doolittle (ref 2), 0.68 g(2)/100 g sln, is available and so no Critical Evaluation is possible. This system clearly requires further investigation.

#### REFERENCES

1. Park, J. G.; Hopkins, M. B. Ind. Eng. Chem. 1930, 22, 826-30.

2. Doolittle, A. K. Ind. Eng. Chem. 1935, 27, 1169-79.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 1-methylpentyl	Park, J.G.; Hopkins, M.B.
ester (1-methylpentyl	Ind. Eng. Chem. <u>1930</u> , 22, 826-30.
acetate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [5953-49-1]	
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EVDEDIMENTAL VALUES.	
The solubility of acetic acid 1-methy	plpentyl ester in water at 25°C was
reported to be less than 0.1 mL(1)/10	00mL(2).
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commer-
	cial samples; used as received; 85-88% of ester, b.p. range
	146-156°C, $n_{\rm D}^{20}$ 1.4081.
	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
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	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Acetic acid 1-methylpentyl	Doolittle, A.K.		
ester (1-methylpentyl	Ind. End. Chem. <u>1935</u> , 27, 1169-79.		
$acecate; c_{8} n_{16} o_2; [5953-49-1]$			
(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 293	A. Skrzecz		
	I		
The solubility of acetic acid 1-methy	ubentul ester in water at 2000 was		
reported to be very slightly soluble.	,		
The solubility of water in acetic aci	id 1-methylpentyl ester at 20 <sup>0</sup> C was		
reported to be 0.68 g(2)/100g sln. Th	ne corresponding mole fraction, $x_2$ ,		
value calculated by the compiler is (	0.052.		
AUXILIARY :	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The method was not specified.	(1) Source not specified, commer-		
	cial product; purity 98%, b.p. range $129-158^{\circ}C$ , $d^{20}$ 0.861.		
	(2) Not specified		
	(2) NOU Specified.		
	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES:		

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COMPONENTS:	EVALUATOR:		
<ul> <li>(1) Butanoic acid butyl ester (butyl butyrate); C<sub>8</sub>H<sub>16</sub>O<sub>2</sub>; [109-21-7]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988		
CRITICAL EVALUATION:			
Quantitative solubility data for the butanoic acid butyl ester (1) - water (2) system have been reported in the publications listed in Table 1.			

TABLE 1:	<u>Quantitative</u> Solubil	<u>ity Studies of the</u>
Butanoic	acid butyl ester (1)	- Water (2) System

	Reference	T/K	Solubility	Method
Bridgman	(ref 1)	283-306	(2) in (1)	synthetic
Doolittle	(ref 2)	293	mutual	unspecified
Chebotaev	et al. (ref 3)	370	(2) in (1)	analytical
Stephenson (ref 4)	n and Stuart	273-364	mutual	GLC

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. SOLUBILITY OF BUTANOIC ACID BUTYL ESTER (1) IN WATER (2)

All the available data for the solubility of butanoic acid butyl ester (1) in water (2) are summarized in Table 2. At 293 K, the only temperature where comparison is possible, the data of Doolittle (ref 2) and Stephenson and Stuart (ref 4) are in serous disagreement. In the absence of independent studies it is impossible to prefer either value although it may be noted that the data of Stephenson and Stuart (ref 4) are generally reliable.

COMPONENTS:	EVALUATOR:
<ul> <li>(1) Butanoic acid butyl ester (butyl butyrate); C<sub>8</sub>H<sub>16</sub>O<sub>2</sub>; [109-21-7]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988
CRITICAL EVALUATION: (continued)	
<u>TABLE 2: Repa</u> of Butanoic acid buty	orted Solubilities 1 ester (1) in Water (2)
T/K R	eported Solubilities
g(1)/100g sln	10 <sup>4</sup> x1 <sup>4</sup>
273 1.22 (ref 4)	15.4
283 0.90 <sup>*</sup> (ref 4)	11.3
293 0.05 (ref 2), 0.66* (ref	4) 8.3
298 0.60 <sup>*</sup> (ref 4)	7.5
303 0.56 <sup>*</sup> (ref 4)	7.0
313 0.52 <sup>*</sup> (ref 4)	6.5
323 0.49 <sup>*</sup> (ref 4)	6.1
333 0.47 <sup>*</sup> (ref 4)	5.9
343 0.47* (ref 4)	5.9
353 0.49 <sup>*</sup> (ref 4)	6.1
363 0.51* (ref 4)	6.3

<sup>a</sup> Data of ref 4, see text.

2. SOLUBILITY OF WATER (2) IN BUTANOIC ACID BUTYL ESTER (1)

All the available data for the solubility of water (2) in butanoic acid butyl ester (1) are summarized in Table 3 with the exception of the value of Chebotaev *et al.* (ref 3) which is much higher than the other (ref 4) study and is rejected. Unlike the  $H_2O$ -rich phase the agreement between independent studies over the range 283-303 is good and a number of values have been Recommended. At other temperatures only the data of Stephenson and Stuart (ref 4) are available, excluding the datum of Chebotaev *et al.* (ref 3) referred to above, and must be considered Tentative pending further studies.

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COMPONENTS:		EVALUATOR:	
(1)	Butanoic acid butyl ester ( <i>butyl butyrate</i> ); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,	
	[109-21-7]	Murdoch University, Perth, W.A.,	
(2) Water; H <sub>2</sub> O; [7732-18-5]		Australia	
		December, 1988	

CRITICAL EVALUATION: (continued)

TABLE	3:	Rec	omm	ende	ed	(R)	and	<u>d Ten</u>	tative	Solub	<u>ilities</u>
of	Wate	er (	2)	in	But	ano	ic	acid	buty1	ester	(1)

T/K	Solubilities				
	Reported values	"Best" values (± $\sigma_r$	n) <sup>a</sup>		
	g(2)/100g sln	g(2)/100g sln	$10^2 x_2$		
273	0.339 (ref 4)	0.34	2.7		
283	0.379 (ref 1), 0.370 <sup>*</sup> (ref 4)	0.37 ± 0.01 (R)	2.9		
293	0.450 <sup>*</sup> (ref 1), 0.43 (ref 2), 0.412 <sup>*</sup> (ref 4)	0.43 ± 0.02 (R)	3.3		
298	0.490 <sup>*</sup> (ref 1), 0.438 <sup>*</sup> (ref 4)	0.46 ± 0.03 (R)	3.5		
303	0.533 <sup>*</sup> (ref 1), 0.466 (ref 4)	0.50 ± 0.03 (R)	3.9		
313	0.53 <sup>*</sup> (ref 4)	0.53	4.1		
323	0.59 <sup>*</sup> (ref 4)	0.59	4.5		
333	0.63 <sup>*</sup> (ref 4)	0.63	4.8		
343	0.66 <sup>*</sup> (ref 4)	0.66	5.1		
353	0.67 <sup>*</sup> (ref 4)	0.67	5.1		
363	0.68 <sup>*</sup> (ref 4)	0.68	5.2		

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_2)$  have the same status and (relative) percentage uncertainties as the mass % solubilities.

# REFERENCES

- 1. Bridgman, J. A. Ind. Eng. Chem. <u>1928</u>, 20, 184-7.
- 2. Doolittle, A. K. Ind. Eng. Chem. <u>1935</u>, 27, 1169-79.
- Chebotaev, V. F.; Balashov, M. I.; Serafimov, L. A. Fiz. Khim. Osn. Rektifikatsii <u>1970</u>, 100-3.
- 4. Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u>, 31, 56-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Butanoic acid butyl ester	Bridgman, J.A.		
(butyl butyrate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ;	Ind. End. Chem. <u>19</u> 28, 20, 184-7.		
[109-21-7]			
(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 283 - 306	Z. Maczynska		
EXPERIMENTAL VALUES:	· · · · · · · · · · · · · · · · · · ·		
Solubility of water in buta	noic acid butyl ester		
$t/^{\circ}C$ g(2)/100g(1) g(2)/1	$x_2$		
(c	ompiler) (compiler)		
10.0 0.380	0.379 0.0296		
16.0 0.424 25.5 0.407	0.422 0.0328		
25.5 0.497	0.494 0.0382		
ΔΙΙΥΤΙ.ΤΔΡΥ	ΤΝΈΟΡΜΔͲΤΟΝ		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The synthetic method similar to that described by Groschuff (ref 1) was used. A glass tube of about 100 mL capacity with a stopcock was filled with weighed (1) and (2). By shaking the tube after it had been	<ul> <li>(1) Source not specified; distil- led; b.p. range 164.5-165.5°C; boiled for some time in open flask before used.</li> <li>(2) Not specified.</li> </ul>		
warmed somewhat, the water was dis- solved completely in the ester,			
after which the tube was placed in a 2-liter beaker filled with water	ESTIMATED ERROR:		
and equipped with an agitator. By	Temp, ±0.25°C.		
it was possible to determine, with- in about 0.5°C, the temperature at which water was precipitated from			
the solution, as shown by the clouding of the liquid which would	REFERENCES:		
clear again when the temperature was slightly increased.	1. Groschuff, E. Z. Elektrochem. <u>1911</u> , 17, 348.		

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Butanoic acid butyl ester	Doolittle, A.K.		
(butyl butyrate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ;	Ind. End. Chem. <u>1935</u> , 27, 1169-79.		
(2) water; H <sub>2</sub> 0; [7/32-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 293	A. Skrzecz		
EXPERIMENTAL VALUES:			
The solubility of butanoic acid butyl	. ester in water at 20 <sup>o</sup> C was reported		
to be 0.05 g(1)/100g sln. The corresp	bonding mole fraction, $x_1$ , value cal-		
culated by the compiler is $6 \times 10^{-5}$ .			
The solubility of water in butanoic a	cid butvl ester at 20°C was reported		
to be 0.43 g(2)/100g sln. The corresp	ponding mole fraction, $x_2$ , value cal-		
culated by the compiler is 0.033.	_		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The method was not specified	(1) Source not specified common		
The method was not specified.	(1) Source not specified, commer- cial product; purity 99%, b.p. range 152-170°C, $d_4^{20}$ 0.874.		
	(2) Not specified.		
	ESTIMATED EDDOD.		
	Not sposified		
	not specified.		
	DEEEDENOEC.		
	REFERENCES:		

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COMPONENTS	5:		ORIGINAL MEASUREMENTS:			
(1) Buta	anoic acid butyl	ester	Stephenson, R.; Stuart, J.			
(but	yl butyrate); C	; <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ;	J. Chem. Eng. Data <u>1986</u> , 31,			
[109	9-21-7]		56-70.			
(2) Wate	er; H <sub>2</sub> O; [7732-1	8-5]				
VARIABLES:			PREPARED BY:			
T/K = 273	3 - 364		Z. Maczynska			
EXPERIMENT	TAL VALUES:		<u> </u>	······································		
И	Mutual solubilit	y of butanoid	c acid butyl ester a	nd water		
t/°C	q(1)/10	0q sln	(qmos) <sub>x</sub>	iler)		
-, -	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase		
0	0.122	99.661	0.000152	0.97349		
9.5	0.102	99.630	0.000127	0.97113		
20.0	0.066	99,560	0.000082	0.96583		
29.7	0.056	99.573	0.000070	0.96681		
39.6	0.052	99.460	0.000065	0.95835		
50.0	0.051	99.423	0.000064	0.95560		
59.9	0.047	99.358	0.000059	0.95082		
70.2	0.047	99.349	0.000059	0.95016		
80.0	0.049	99.320	0.000061	0.94804		
90.3	0.051	99.317	0.000064	0.94782		
std. de	. 0.001	0 004				
Jul u		0.004				
		AUXILIARY	INFORMATION			
METHOD/APP	ARATUS/PROCEDUR	E:	SOURCE AND PURITY	OF MATERIALS:		
The analy	tical mothod wa	a ugod	(1) Course not exception common			
Component	(1) was equili	brated	cial sample; ]	purity 99%; used		
with comp	onent (2) at a re in a thermos	given tat. Each	as received.			
layer was	sampled with a	syringe;	(2) Not specified.			
(1) was d weighed a	etermined by ad	ding a itrile				
(or somet	imes propanol)	to the				
organic l by a Gow-	ayer sample and Mac thermal con	measuring ductivitv	ESTIMATED ERROR:			
gc the (1	)/acetonitrile	peak ratio	Accuracy of mother	10.1 wts or loss		
(Chromoso 3390 A re	rb 101 packing corder-integrat	and a HP or).	for solubility, se	e above.		
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the						
water lay	er.		REFERENCES:			
		(				

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COMPONE	NTS:		ORIGINAL MEASUREMENTS:			
(1) Fe	ormic acid hepty	l ester	Stephenson, R.; Stuart, J.			
(1	heptyl formate);	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ;	J. Chem. Eng. Dat	a <u>1986</u> , 31,		
[ [:	112-23-2]		56-70.			
(2) Wa	ater; H <sub>2</sub> O; [7732-	-18-5]				
VARIABL	ES:		PREPARED BY:			
T/K = 3	273 - 364		Z. Maczynska			
EXPERIM	ENTAL VALUES:		k			
	Mutual solubili	ity of formic a	acid heptyl ester ar	nd water		
t/°c	α(1)/1	00g sln	X. (Comp	iler)		
	(2)-rich phase	e (1)-rich phas	se (2)-rich phase	(1)-rich phase		
0	-	99.32	-	0.9480		
9.1	-	99.37	-	0.9517		
19.5	0.162	99.32	0.000203	0.9480		
29.7	0.142	-	0.000178	-		
39.6	0.078	99.20	0.000097	0.9393		
50.0	0.071	99.15	0.000089	0.9358		
60.1	0.063	98.88	0.000079	0.9168		
70.1	0.087	98.94	0.000109	0.9210		
80.0	0.075	98.92	0.000094	0.9196		
90.6	0.056	98.81	0.000070	0.9120		
std.	dev. 0.002	0.01				
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		AUXILIARY	INFORMATION			
METHOD/	APPARATUS/PROCEDU	JRE:	SOURCE AND PURITY	OF MATERIALS:		
The ana	alytical method w	as used.	(1) Source not specified, commer-			
Compone with co	ent (1) was equil omponent (2) at a	ibrated given	cial sample; purity 97%; used as received.			
tempera	ture in a thermo	stat. Each				
(1) was	as sampled with determined by a	a syringe; adding a	(2) Not specified.			
weighed	amount of aceto	nitrile				
organic	c layer sample an	d measuring	ESTIMATED ERROR:			
gc the	(1)/acetonitrile	e peak ratio				
(Chromosorb 101 packing and a HP			for solubility, see above.			
A simil	lar procedure but	a higher				
boiling material (e.g. 1-hexanol) was used to determine (2) in the			·····			
water layer.			REFERENCES:			
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COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Heptanoic acid methyl ester			Stephenson, R.; Stuart, J.		
(methyl enanthate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [106-73-0]		J. Chem. Eng. Data <u>1986</u> , 31, 56-70.			
(2) Wate	er; H <sub>2</sub> O; [7732-1	.8-5]			
VARIABLES:			PREPARED BY:		
T/K = 273 - 364			Z. Maczynska		
EXPERIMENTAL VALUES:			L		
Mu	utual solubility	of heptanoic	acid methyl ester	and water	
$t/^{\circ}C$ g(1)/100g sln			x <sub>1</sub> (compiler)		
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase	
0	0.105	99.45	0.000131	0.9576	
9.5	0.122	99.42	0.000152	0.9554	
19.3	0.094	99.33	0.000117	0.9488	
30.0	0.090	99.30	0.000112	0.9466	
39.6	0.063	99.36	0.000079	0.9509	
49.8	-	99.24	-	0.9422	
60.5	0.054	99.27	0.000067	0.9444	
70.5	0.087	99.28	0.000109	0.9451	
80.5	0.066	99.24	0.000082	0.9422	
90.5	0.053	99.13	0.000066	0.9343	
std. de	ev. 0.001	0.01			
		AUXILIARY 1	INFORMATION		
METHOD/APP	PARATUS/PROCEDUR	E:	SOURCE AND PURITY	OF MATERIALS:	
The analy Component	vtical method wa : (1) was equili	s used. brated	(1) Source not specified, commer- cial sample; purity 99%; used		
with comp	onent (2) at a	given tat Each	as received.		
layer was	sampled with a	syringe;	(2) Not specified.		
<pre>(1) was d weighed a</pre>	letermined by ad mount of aceton	ding a itrile			
(or somet	imes propanol)	to the			
by a Gow-	Mac thermal con	ductivity	ESTIMATED ERROR:		
gc the (1	)/acetonitrile	peak ratio	Accuracy of metho	d 0.1 wt% or less.	
3390 A re	corder-integrat	or).	for solubility, s	ee above.	
A similar	procedure but	a higher			
was used	to determine (2	) in the			
water lay	er.		REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ul> <li>(1) Hexanoic acid ethyl ester (ethyl caproate); C<sub>8</sub>H<sub>16</sub>O<sub>2</sub>; [123-66-0]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	Sobotka, H.; Kahn, J. J. Am. Chem. Soc. <u>1931</u> , 53, 2935-8.	
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES:	·	

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The solubility of hexanoic acid ethyl ester in water at  $20^{\circ}C$  was reported to be 0.063 g(1)/100mL(2). The corresponding mass per cent and mole fraction,  $x_1$ , values calculated by the compiler are 0.063 g(1)/100g sln and 7.9 x  $10^{-5}$ .

Density of water  $d_4^{20} = 0.9982$  (ref 1) was used in the calculation.

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent droplets.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified (Eastman Kodak Laboratories or synthe- sized); twice-distilled under reduced pressure; n<sup>D</sup><sub>D</sub> 1.4089. (2) Distilled. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES: 1. Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, 1973.</pre>			

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Hexanoic acid ethyl ester	Stephenson, R.; Stuart, J.		
(ethyl caproate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ;	J. Chem. Eng. Data <u>1986</u> , 31, 56-70.		
(2) Water: $H_0$ : $(7732-18-5)$			
VARIABLES:	PREPARED DI:		
T/K = 273 - 364	Z. Maczynska		
EXPERIMENTAL VALUES:			
Mutual solubility of nexano	ic acid etnyi ester and water		
t/ <sup>o</sup> C g(1)/100g sln	$x_1$ (compiler)		
(2)-rich phase (1)-rich pha	se (2)-rich phase (1)-rich phase		
0 0.107 99.64	0.000134 0.9719		
9.6 0.102 99.61	0.000127 0.9696		
19.7 0.083 99.53	0.000104 0.9636		
29.6 0.075 99.49	0.000094 0.9606		
39.8 0.070 99.44	0.000087 0.9568		
50.0 0.060 99.42	0.000075 0.9554		
60.6 0.049 99.38	0.000061 0.9524		
70.5 0.055 99.34	0.000069 0.9495		
80.4 0.055 99.29	0.000069 0.9458		
90.6 0.059 99.26	0.000074 0.9437		
std. dev. 0.007 0.01			
AUXILIARY	INFORMATION		
	SOURCE AND DURTTY OF MATERIALS.		
	SOURCE AND FURTH OF MATERIALS.		
The analytical method was used. Component (1) was equilibrated with component (2) at a given	(1) Source not specified, commer- cial sample; purity 99%; used as received.		
temperature in a thermostat. Each	(2) Not specified		
(1) was determined by adding a			
(or sometimes propanol) to the			
organic layer sample and measuring	ESTIMATED ERROR:		
gc the (1)/acetonitrile peak ratio			
(Chromosorb 101 packing and a HP	Accuracy of method 0.1 wt% or less, for solubility, see above.		
A similar procedure but a higher			
boiling material (e.g. 1-hexanol)			
water layer.	REFERENCES:		

				119	
COMPONENTS:			ORIGINAL MEASUREMEN	NTS:	
(1) Propa	noic acid, 2-	methyl-,	Stephenson, R.; Stuart, J.		
butyl	lester		J. Chem. Eng. Data	1986. 31.	
(buty	/l isobutyrate	); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ;	56-70.	<u>1900</u> , 91,	
[9/-8	37-01				
(2) Water	; H <sub>2</sub> O; [7732-	18-5]			
VARIABLES:			PREPARED BY:	, ,	
T/K = 273 - 364			Z. Maczynska		
	T WATUEC.		<u> </u>	·····	
Mutual	solubility of	2-methylprop	anoic acid butyl este	er and water	
t/°C	g(1)/1	00g sln	$x_1$ (compi	ler)	
(	2)-rich phase	(1)-rich pha	se (2)-rich phase	(1)-rich phase	
<u> </u>	0,090	99,64	0,000112	0.9719	
9.8	0.071	99.63	0.000089	0.9711	
19.6	0.077	99.57	0.000096	0.9666	
30.9	0.076	99.61	0.000095	0.9696	
40.1	0.051	99.53	0.000064	0.9636	
50.0	0.043	99.51	0.000054	0.9621	
60.0	0.048	99.42	0.000060	0.9554	
70.0	0.043	99.34	0.000054	0.9495	
80.2	0.044	99.35	0.000055	0.9502	
90.5	0.043	99.32	0.000054	0.9480	
std. dev	. 0.003	0.01			
	· · · · · · · · · · · · · · · · · · ·	AUXILIARY	INFORMATION		
METHOD/APPA	RATUS/PROCEDU	RE:	SOURCE AND PURITY O	F MATERIALS:	
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a		<ul> <li>(1) Source not special sample; pas received.</li> <li>(2) Not specified.</li> </ul>	cified, commer- urity 98%; used		
weighed am (or sometime	ount of acetor mes propanol)	itrile to the			
organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol)		ESTIMATED ERROR:			
		Accuracy of method for solubility, se	0.1 wt% or less, e above.		
water laye	r.	, <u>11</u> 0110	REFERENCES:		
				· · · · · · · · · · · · · · · · · · ·	

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COMPONENTS:			ORIGINAL MEASUREMENT	rs:				
(1) Propanoic acid 3-methyl-			Stephenson, R.; Stuart, J.					
1-butyl ester ( <i>isopentyl propionate</i> ); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [105-68-0]		J. Chem. Eng. Data <u>1986</u> , 31, 56-70.						
				(2) Water	; H <sub>2</sub> O; [7732-	18-5]		
				VARIABLES: T/K = 273 - 364			PREPARED BY:	
Z. Maczynska								
EXPERIMENTA	L VALUES:	<u></u>	I					
Mutual s	olubility of	propanoic ació	d 3-methyl-1-butyl es	ter and water				
t/°C	g(1)/1	00g sln	$x_1$ (compil	ler)				
(	2)-rich phase	(1)-rich phas	se (2)-rich phase (2	1)-rich phase				
0	0.097	99.57	0.000121	0.9666				
9.3	0.100	99.57	0.000125	0.9666				
19.3	0.065	99.52	0.000081	0.9628				
29.7	0.056	99.46	0.000070	0.9583				
40.0	0.063	99.40	0.000079	0.9539				
49.8	0.045	99.47	0.000056	0.9591				
60.0	0.056	99.40	0.000070	0.9539				
70.0	0.075	-	0.000094	-				
79.7	0.057	99.22	0.000071	0.9408				
90.6	0.064	99.68	0.000080	0.9032				
std. dev	. 0.001	0.01						
		AUXILIARY	INFORMATION					
ETHOD/APPAI	RATUS/PROCEDU	RE:	SOURCE AND PURITY OF	MATERIALS:				
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe:			(1) Source not specified, commer- cial sample; purity 99%; used as received.					
			(2) Not specified.					
(1) was det weighed amo	termined by a ount of aceto	dding a nitrile						
(or sometimes propanol) to the organic layer sample and measuring								
by a Gow-Ma	ac thermal co	nductivity	ESTIMATED ERROR:					
gc the (1), (Chromosori 3390 A reco A similar p boiling mat	b 101 packing order-integra procedure but terial (e.g.	peak ratio and a HP tor). a higher 1-hexanol)	Accuracy of method for solubility, see	0.1 wt% or less above.				
was used to	o determine (	2) in the						
acer rayer	- •		REFERENCES:					

OMPONENTS: (1) Propanoic acid, 2-methyl-, 2-methylpropyl ester (isobutyl isobutyrate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ; [97-85-8]			ORIGINAL MEASUREMEN Stephenson, R.; St J. Chem. Eng. Data 56-70.	NTS: tuart, J. a <u>1986</u> , 31,		
(2) Wate	r; H <sub>2</sub> O; [7732-	-18-5]				
RIABLES:			PREPARED BY:	•		
V/K = 273	- 363		Z. Maczynska	Z. Maczynska		
·	(2)-rich phase	> (1)-rich ph	ase (2)-rich phase	(1)-rich phase		
		• ••••••••••••••••••••••••••••••••••••		<u></u>		
		QQ 57	0 000122	~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~		
0	0.098	55.57	0.000122	0.9666		
0 9.3	0.098	99.48	-	0.9598		
0 9.3 19.4	0.098 - 0.050	99.48 99.46	0.000062	0.9598 0.9583		
0 9.3 19.4 29.6 39.5	0.098 - 0.050 0.049	99.48 99.46 99.29	- 0.000062 0.000061	0.9666 0.9598 0.9583 0.9458		
0 9.3 19.4 29.6 39.5 50.0	0.098 - 0.050 0.049 0.050 0.051	99.48 99.46 99.29 99.43 99.40	- 0.000062 0.000061 0.000062 0.000064	0.9666 0.9598 0.9583 0.9458 0.9561 0.9539		
0 9.3 19.4 29.6 39.5 50.0 59.8	0.098 - 0.050 0.049 0.050 0.051 0.046	99.48 99.46 99.29 99.43 99.40 99.18	- 0.000062 0.000061 0.000062 0.000064 0.000057	0.9666 0.9598 0.9583 0.9458 0.9561 0.9539 0.9379		
0 9.3 19.4 29.6 39.5 50.0 59.8 70.2	0.098 - 0.050 0.049 0.050 0.051 0.046 0.045	99.48 99.46 99.29 99.43 99.40 99.18 99.26	- 0.000062 0.000061 0.000062 0.000064 0.000057 0.000056	0.9666 0.9598 0.9583 0.9458 0.9561 0.9539 0.9379 0.9437		
0 9.3 19.4 29.6 39.5 50.0 59.8 70.2 80.1	0.098 - 0.050 0.049 0.050 0.051 0.046 0.045 0.041	99.48 99.46 99.29 99.43 99.40 99.18 99.26 99.24	- 0.000062 0.000061 0.000062 0.000064 0.000057 0.000056 0.000051	0.9666 0.9598 0.9583 0.9458 0.9561 0.9539 0.9379 0.9437 0.9422		
0 9.3 19.4 29.6 39.5 50.0 59.8 70.2 80.1 90.3	0.098 - 0.050 0.049 0.050 0.051 0.046 0.045 0.041 0.056	99.48 99.46 99.29 99.43 99.40 99.18 99.26 99.24 99.20	- 0.000062 0.000061 0.000062 0.000064 0.000057 0.000056 0.000051 0.000070	0.9666 0.9598 0.9583 0.9458 0.9561 0.9539 0.9379 0.9437 0.9422 0.9393		
0 9.3 19.4 29.6 39.5 50.0 59.8 70.2 80.1 90.3 std. dev	0.098 - 0.050 0.049 0.050 0.051 0.046 0.045 0.041 0.056 7. 0.001	99.48 99.46 99.29 99.43 99.40 99.18 99.26 99.24 99.20 0.02	- 0.000062 0.000061 0.000062 0.000064 0.000057 0.000056 0.000051 0.000051	0.9666 0.9598 0.9583 0.9458 0.9561 0.9539 0.9379 0.9437 0.9422 0.9393		

# METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial sample; purity 98%; used as received.
- (2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

**REFERENCES:** 

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Propanoic acid pentyl ester	Hemptinne, A.	
(pentyl propionate); C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> ;	Z. Phys. Chem. <u>1894</u> , 13, 561-9.	
[624-54-4]		
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of propanoic acid pent	yl ester in water at 25 <sup>°</sup> C was report-	
ed to be 0.908 g(1)/L sln.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The analytical method was used. The	(1) Not specified.	
mixture of water with excess ester was beated for some time in a water	(2) Not specified	
bath and the ester phase was fil-		
was then transferred to a smaller		
flask, heated with the known amount of baryta until complete saponifi-		
cation was obtained and then ti- trated. No further details were re-	ESTIMATED ERROR:	
ported in the paper.	Not specified.	
	-	
	DEFEDENCES.	
	REFERENCED.	

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 2-butoxyethyl	Doolittle, A.K.
ester (2-butoxyethyl acetate);	Ind. End. Chem. <u>1935</u> , 27, 1169-79.
$C_8H_{16}O_3; [112-07-2]$	
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES:	de
The solubility of acetic acid 2-butos	wethyl ester in water at 20°C was
reported to be 0.9 g(1)/100g sln. The	e corresponding mole fraction, $x_1$ ,
value calculated by the compiler is (	0.0010.
The solubility of water in acetic act	id 2-butoxyethyl ester at 20°C was
reported to be 1.9 g(2)/100g sln. The	e corresponding mole fraction, $x_2$ ,
value calculated by the compiler is (	0.15.
AUXILIARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commer-
	range $188-192^{\circ}C$ , $d_4^{20}$ 0.943.
	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

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COMPONENTS:		EVALUATOR:	
(1)	Acetic acid phenylmethyl ester ( <i>benzyl acetate</i> ); C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,	
	[140-11-4]	Murdoch University, Perth, W.A.,	
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988	

CRITICAL EVALUATION:

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

TABLE 1: Quantitative Solubility Studies of the Acetic acid phenylmethyl ester (1) - Water (2) System				
Reference	Т/К	Solubility	Method	
Goto et al. (ref 1)	363	(1) in (2)	GLC	
Stephenson and Stuart (ref 2)	273-364	mutual	GLC	

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. SOLUBILITY OF ACETIC ACID PHENYLMETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid phenylmethyl ester (1) in water (2) are summarized in Table 2. At 363 K, the only temperature where comparison is possible, the data of Goto *et al.* (ref 1) and Stephenson and Stuart (ref 2) are in fair agreement. At other temperatures only the data of Stephenson and Stuart (ref 2) are available and in the absence of other studies must be regarded as Tentative, although it may be noted that the solubilities reported by these authors are usually reliable.

COMPONENTS:		EVALUATOR:	
(1)	Acetic acid phenylmethyl ester ( <i>benzyl acetate</i> ); C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,	
	[140-11-4]	Murdoch University, Perth, W.A.,	
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988	

CRITICAL EVALUATION: (continued)

## TABLE 2: Tentative Solubilities of Acetic acid phenylmethyl ester (1) in Water (2)

T/K	Solubilit	ies	
	Reported values	"Best" values	a
	g(1)/100g sln	g(1)/100g sln	10 <sup>4</sup> x <sub>1</sub>
273	0.253 (ref 2)	0.25	3.0
283	0.253 (ref 2)	0.25	3.0
293	0.255 <sup>*</sup> (ref 2)	0.26	3.1
298	0.258 <sup>*</sup> (ref 2)	0.26	3.1
303	0.262 <sup>*</sup> (ref 2)	0.26	3.1
313	0.277 <sup>*</sup> (ref 2)	0.28	3.3
323	0.305 <sup>*</sup> (ref 2)	0.31	3.6
333	0.338 <sup>*</sup> (ref 2)	0.34	4.0
343	0.372 <sup>*</sup> (ref 2)	0.37	4.5
353	0.409 (ref 2)	0.41	4.9
363	0.58 (ref 1), 0.447* (ref 2)	0.45	5.4

<sup>a</sup> Rounded values of ref 2, see text.

# 2. SOLUBILITY OF WATER (2) IN ACETIC ACID PHENYLMETHYL ESTER (1)

The only data available for the solubility of water (2) in acetic acid phenylmethyl ester (1) are those of Stephenson and Stuart (ref 2) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental results but it may be noted that solubilities reported by these authors are usually reliable.

#### REFERENCES

- Goto, S.; Matsubara, M.; Washino, K. Kagaku Kogaku <u>1974</u>, 38, 869-73.
- 2. Stephenson, R.; Stuart, J. J. Chem. Eng. Data 1986, 31, 56-70.

-20				
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Acetic acid phenylmethyl ester (benzyl acetate); C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ; [140-11-4]	Goto, S.; Matsubara, M.; Washino, K. Kagaku Kogaku 1974. 38(12).			
(2) Water; $H_2O$ ; [7732-18-5]	869-73.			
VARIABLES:	PREPARED BY:			
T/K = 363	A. Skrzecz			
EXPERIMENTAL VALUES: The solubility of acetic acid phenylm reported to be 0.57 and 0.58 g(1)/100 fraction, $x_1$ , value calculated by the	hethyl ester in water at 90°C was og sln. The corresponding mole a compiler is 6.9 x 10 <sup>-4</sup> .			
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The analytical method was used. The samples of total volume about 50 cm <sup>3</sup> containing acetic acid phenylmethyl ester, water and tetralin were thermostated at 90°C, mixed and separated over 1 h. Then, the phases were ana- lysed by glc. The method and data were reported together with the	<ul> <li>(1) Source not specified; purity &gt;99 wt%; used as received.</li> <li>(2) Distilled.</li> </ul>			
ternary system acetic acid phenyl- methyl ester-water-tetralin. Tetralin was not detected in the water phase.	Soly. <±0.01 g(1)/100g sln (compiler).			
	REFERENCES:			

			y		
COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Acetic acid phenylmethyl ester			Stephenson, R.; Stuart, J.		
(benzyl acetate); C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ;			J. Chem. Eng. Data	a 1986, <i>31</i> ,	
[140-11-4]			56-70.		
(2) Water; H <sub>2</sub> O; [7732-18-5]					
VARIABLES:			PREPARED BY:		
T/K = 273 -	364		Z. Maczynska		
				· · · · · · · · · · · · · · · · · · ·	
EXPERIMENTAL Mutual	VALUES: solubility	of acetic acid	d phenylmethyl ester	and water	
	a(1)/1				
(2	)-rich phase	(1)-rich phas	$x_1$ (complete set (2)-rich phase	(1)-rich phase	
	,	(_,			
0	0.253	99.38	0.000304	0.9506	
9.7	0.253	99.36	0.000304	0.9490	
20.0	0.266	99.22	0.000320	0.9385	
30.7	0.240	99.08	0.000288	0.9281	
40.3	0.278	98.94	0.000334	0.9180	
49.8	0.305	98.79	0.000367	0.9073	
60.1	0.336	98.61	0.000404	0.8948	
70.4	0.375	98.41	0.000451	0.8813	
80.1	0.409	98.17	0.000492	0.8655	
90.4	0.448	97.83	0.000539	0.8439	
std. dev.	0.002	0.03			
			······································		
		AUXILIARY I	INFORMATION		
METHOD/APPAR	ATUS/PROCEDU	RE:	SOURCE AND PURITY C	OF MATERIALS:	
The analytic	cal method wa	as used.	<ul> <li>(1) Source not specified, commer- cial sample; purity 99%; used as received.</li> <li>(2) Not specified.</li> </ul>		
Component (	1) was equil: ent (2) at a	ibrated given			
temperature	in a thermos	stat. Each			
(1) was det	ampled with a ermined by a	a syringe; dding a			
weighed amon	weighed amount of acetonitrile				
(or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP					
			ESTIMATED ERROR:		
			Accuracy of method 0.1 wt% or less,		
3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.		tor solubility, se	e above.		
		DEFEDENCES.	·····		
		Kelekences:			
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COMPONENTS:	EVALUATOR:
<ol> <li>Benzoic acid ethyl ester</li> <li>(ethyl benzoate); C<sub>9</sub>H<sub>10</sub>O<sub>2</sub>;</li> </ol>	G.T. Hefter, School of Mathematical and Physical Sciences,
[93-89-0]	Murdoch University, Perth, W.A.,
(2) Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988

CRITICAL EVALUATION:

Stephenson and Stuart

(ref 2)

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

	<u>TABLE 1: Qu</u> <u>Benzoic aci</u>	antitative Solu) 1 ethyl ester (1	<u>ntitative Solubility Studies of the</u> ethyl ester (1) - Water (2) System		
	Reference	T/K	Solubility	Method	
Krupatkin (ref 1)	and Glagoleva	298	mutual	titration	

273-363

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.

mutual

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1. SOLUBILITY OF BENZOIC ACID ETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of benzoic acid ethyl ester (1) in water (2) are summarized in Table 2. At 298 K, the only temperature where comparison is possible, the data of Krupatkin and Glagoleva (ref 1) and Stephenson and Stuart (ref 2) are in only fair agreement. At other temperatures only the data of Stephenson and Stuart (ref 2) are available. Although the data reported by these authors are usually reliable their results for the present system are very scattered and, pending further studies, should be regarded as very Tentative.

COMPC	DNENTS:	EVALUATOR:	
(1)	Benzoic acid ethyl ester ( <i>ethyl benzoate</i> ); C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ; [93-89-0] Water; H <sub>2</sub> O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988	
CRITI	CAL EVALUATION: (continued)		
	<u>TABLE 2: Tenta</u> of Benzoic acid ethyl	<u>ttive Solubilities</u> ester (1) in Water (2)	
т/к	Sol	lubilities	
	Reported values	"Best" values <sup>a</sup>	
	g(1)/100g sln	g(1)/100g sln $10^4 x_1$	
273	0.108 (ref 2)	0.1 1	
283	0.095 <sup>*</sup> (ref 2)	0.1 1	
293	0.085 <sup>*</sup> (ref 2)	0.09 1	
298	0.15 <sup>b</sup> (ref 1), 0.085 <sup>*</sup> (ref	2) 0.09 1	
303	0.090 (ref 2)	0.09 1	
313	0.10 <sup>*</sup> (ref 2)	0.1 1	
323	0.11 <sup>*</sup> (ref 2)	0.1 1	
333	0.11 <sup>*</sup> (ref 2)	0.1 1	

<sup>a</sup> Rounded values of ref 2, but see text.

0.12\* (ref 2)

0.13<sup>\*</sup> (ref 2)

0.14<sup>\*</sup> (ref 2)

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j,

<sup>b</sup> Not included in estimation of "Best" value.

2. SOLUBILITY OF WATER (2) IN BENZOIC ACID ETHYL ESTER (1)

All the available data for the solubility of water (2) in benzoic acid ethyl ester (1) are summarized in Table 3. The situation for the organicrich phase is equivalent to that of the  $H_2O$ -rich phase and the user is referred to the comments in Part 1. of this Evaluation.

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0.1

0.1

(continued next page)

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COMPONENTS:	EVALUATOR:		
<ul> <li>(1) Benzoic acid ethyl ester (<i>ethyl benzoate</i>); C<sub>9</sub>H<sub>10</sub>O<sub>2</sub>; [93-89-0]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988		
CRITICAL EVALUATION: (continued)			
<u>TABLE 3: Tentat</u> of Water (2) in Benzoi	<u>ive Solubilities</u> c acid ethyl ester (1)		
T/K Sol	ubilities		
Reported values	"Best" values <sup>a</sup>		
g(2)/100g sln	g(2)/100g sln	$10^2 x_2$	
283 1.1 <sup>*</sup> (ref 2)	1.1	8	
293 1.0 <sup>*</sup> (ref 2)	1.0	7	
298 $0.57^{b}$ (ref 1), $1.0^{*}$ (ref 2)	1.0	7	
303 0.9 <sup>*</sup> (ref 2)	0.9	7	
313 0.9 <sup>*</sup> (ref 2)	0.9	7	
323 1.1 <sup>*</sup> (ref 2)	1.1	8	
333 1.0 <sup>*</sup> (ref 2)	1.0	7	
a Rounded values of ref 2, but see t	ext.		
<sup>b</sup> Not included in calculation of "Be	st" value.		
REFERENCES			
<ol> <li>Krupatkin, I. L.; Glagoleva, M. 1795-9.</li> </ol>	F. Zh. Prikl. Khim. <u>1972</u> ,	45,	
2. Stephenson, R.; Stuart, J. J. C	hem. Eng. Data <u>1986</u> , 31, 5	6-70.	
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	······		
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COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) Benzoic acid ethyl ester (ethyl benzoate); C<sub>9</sub>H<sub>10</sub>O<sub>2</sub>; [93-89-0]</pre>	Krupatkin, I.L.; Glagoleva, M.F. <i>Zh. Prikl. Khim.</i> <u>1972</u> , 45, 1795-9.		
(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 298	A. Skrzecz		
EXPERIMENTAL VALUES: The solubility of benzoic acid ethyl to be 0.15 g(1)/100g sln. The corresp culated by the compiler is 1.8 x 10 <sup>-4</sup> The solubility of water in benzoic ac to be 0.57 g(2)/100g sln. The corresp culated by the compiler is 0.046.	ester in water at $25^{\circ}$ C was reported ponding mole fraction, $x_1$ , value cal- cid ethyl ester at $25^{\circ}$ C was reported ponding mole fraction, $x_2$ , value cal-		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The titration method was used as described in the publication of Krupatkin and Glagoleva (ref 1). The samples were titrated up to turbidity. The data were reported together with the ternary system benzoic acid ethyl ester-water- 2-furancarbonal (ethyl benzoater	<ol> <li>Source not specified; b.p. 212°C, d<sup>25</sup><sub>25</sub> 1.050, n<sup>25</sup><sub>D</sub> 1.5050.</li> <li>Twice distilled.</li> </ol>		
water-furfural). No further details were reported in the paper.	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES:		
	1. Krupatkin, I.L.; Glagoleva, M.F. Zh. Prikl. Khim. <u>1969</u> , 42, 880.		

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COMPONENT	S:		ORIGINAL MEASUREME	ENTS:	
(1) Benzoic acid ethyl ester		Stephenson, R.; Stuart, J.			
(ethyl benzoate); C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ; [93-89-0]		J. Chem. Eng. Data <u>1986</u> , 31, 56-70.			
(2) Wat	er; H <sub>2</sub> O; [7732-1	.8-5]			
VARIABLES	:		PREPARED BY:		
T/K = 27	3 - 363		Z. Maczynska		
EXPERIMEN	TAL VALUES:	<u>,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,</u>	I		
1	Mutual solubili	cy of benzoic	acid ethyl ester an	nd water	
$t/^{\circ}C$ $q(1)/100q sln$		$x_1$ (comp	oiler)		
	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase	
0	0.108	98.81	0.000130	0.9088	
9.5	-	99.18	-	0.9355	
19.6	0.085	99.01	0.000102	0.9230	
30.5	0.081	99.08	0.000097	0.9281	
40.0	0.106	99.02	0.000127	0.9238	
50.0	0.108	98.88	0.000130	0.9137	
60.1	0,117	98.97	0.000140	0.9202	
70.5	0.121	-	0.000145	-	
80.2	0.121	-	0.000145	-	
90.3	0.143		0.000172	-	
std. de	ev. 0.002	0.01			
		AUXILIARY	INFORMATION		
METHOD / API	PARATUS / PROCEDU	2E.	SOURCE AND PURTTY	OF MATERIALS!	
Component with com	(1) was equili conent (2) at a	ls used. brated given	(1) Source not specified, commer- cial sample; purity 97%; used as received		
temperati	ire in a thermos	stat. Each			
layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity		(2) NOT Specified			
			_		
		ESTIMATED ERROR:			
gc the () (Chromoso	brb 101 packing	peak ratio and a HP	Accuracy of method 0.1 wt% or less,		
3390 A re	ecorder-integrat	.or).	for solubility, s	ee above.	
boiling n	aterial (e.g. 1	-hexanol)			
was used to determine (2) in the		······································			
water Ig	CT.		REFERENCES:		

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COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Benzoic acid, 2-hydroxy-,		Stephenson, R.; S	tuart, J.		
ethyl ester		J. Chem. Eng. Dat	a <u>1986</u> , 31,		
	I O · [119-61-6]	,	56-70.		
Cg1	1003, [118-01-0]		[		
(2) Wat	ter; H <sub>2</sub> O; [7732-	18-5]			
VARIABLES	TABLES: PREPARED BY:				
T/K = 27	73 - 364		Z. Maczynska		
EXPERIMEN	TAL VALUES:		I		
Muti	al solubility o	f 2-hydroxyber	nzoic acid ethyl est	er and water	
t/°C	q(1)/1		X1 (COM)	iler)	
	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase	
				······	
0	-	99.80	-	0.9818	
9.2	0.067	99.76	0.000073	0.9783	
19.5	0.036	99.79	0.000039	0.9809	
29.8	0.037	99.68	0.000040	0.9712	
39.7	0.029	99.74	0.000031	0.9765	
49.8	0.050	99.73	0.000054	0.9756	
60.1	0.040	99.76	0.000043	0.9783	
70.1	0.040	99.54	0.000043	0.9591	
80.1	0.069	99.37	0.000075	0.9447	
90.5	0.078	99.33	0.000085	0.9414	
std. dev. 0.003 0.01					
		AUXILIARY .			
METHOD/AF	PPARATUS/PROCEDU	RE:	SOURCE AND PURITY OF MATERIALS:		
The anal	ytical method wa	as used.	(1) Source not specified, commer-		
with com	ponent (2) at a	given	as received.	purity 97%; used	
temperat	ure in a thermos	stat. Each	(2) Not specified.		
(1) was	determined by a	lding a			
weighed	weighed amount of acetonitrile				
organic layer sample and measuring					
by a Gow qc the (	by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP		ESTIMATED ERROR:		
(Chromos			Accuracy of metho for solubility, s	d 0.1 wt% or less, ee above.	
A simila	r procedure but	a higher	,		
boiling	material (e.g.	L-hexanol)			
was used Water la	yer.	, in the	REFERENCES:		

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COMPONENTS:	EVALUATOR:
<ul> <li>(1) 1,2,3-Propanetriol triacetate</li> <li>(glycerol triacetate); C<sub>9</sub>H<sub>14</sub>O<sub>6</sub>;</li> <li>[102-76-1]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
	December, 1988

CRITICAL EVALUATION:

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

<u>TABLE 1: Quantitative Solubility Studies of the</u> <u>1,2,3-Propanetriol triacetate (1) - Water (2) System</u>			
Reference	T/K	Solubility	Method
Othmer et al. (ref 1)	297 <sup>a</sup>	mutual	unspecified
Kraus et al. (ref 2)	298	mutual	analytical, Karl Fischer

<sup>a</sup> 23.5 <sup>o</sup>C.

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation and are summarized in Tables 2 and 3 below. Unfortunately, these two independent studies are in poor agreement in both the  $H_2O$ -rich and the organic-rich phases (the slight temperature difference should not be important) and the average "Best" values must be regarded as very Tentative, pending further studies.

## TABLE 2: Tentative Solubilities of 1,2,3-Propanetriol triacetate (1) in Water (2)

г/к	Solubilities			
	Reported values	"Best" value <sup>a</sup>		
	g(1)/100g sln	g(1)/100g sln	$10^{3}x_{1}$	
298	5.5 <sup>b</sup> (ref 1), 7.4 (ref 2)	6.5 ± 1.0	5.7	

<sup>a</sup> Average value, but see text.  $x_1$  has the same (relative) percentage uncertainty as the mass % solubility.

<sup>b</sup> 296.7 К.

(continued next page)

COMPONENTS:		EVALUATOR:			
(1) 1,2,3-Pro (glycerol [102-76-1	panetriol triacetate ! <i>triacetate</i> ); C <sub>9</sub> H <sub>14</sub> O <sub>6</sub> ; ]	G.T. Hefter, School of M and Physical Sciences, Murdoch University, Pert	Mathematical		
(2) Water; H <sub>2</sub>	0; [7732-18-5]	December, 1988			
CRITICAL EVALUA	CRITICAL EVALUATION: (continued)				
			·		
<u></u>	<u>TABLE 3: Tentat</u> <u>f Water (2) in 1,2,3-Pro</u>	<u>ive Solubilities</u> ppanetriol_triacetate_(1)			
T/K	Sol	lubilities			
	Reported values	"Best" value <sup>2</sup>	ł		
	g(2)/100g sln	g(2)/100g sln	<i>x</i> <sub>2</sub>		
298 2.5 <sup>b</sup>	(ref 1), 4.60 (ref 2)	3.5 ± 1.0	0.31		
<sup>a</sup> Average val percentage	ue, but see text. $x_2$ luncertainty as the mass	has the same status and (r % solubility.	elative)		
<sup>b</sup> 296.7 К.					
REFERENCES					
1. Othmer, D. 1240-8.	F.; White, R. E.; Tr	ueger, E. Ind. Eng. Chem.	<u>1941</u> , 33,		
2. Kraus, K. 86, 2571-6	A.; Rardon, R. J.; Ba ·	ldwin, W. H. J. Am. Chem.	Soc. <u>1964</u> ,		

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1,2,3-Propanetriol triacetate  (glycerol triacetate); C<sub>9</sub>H<sub>14</sub>O<sub>6</sub>;  [102-76-1]</pre>	Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. <u>1941</u> , 33, 1240-8.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of 1,2,3-propanetriol ported to be 5.5 g(1)/100g sln. The c calculated by the compiler is 0.0048. The solubility of water in 1,2,3-prop ported to be 2.5 g(2)/100g sln. The c calculated by the compiler is 0.24.	triacetate in water at 24.5°C was re- corresponding mole fraction, $x_1$ , value panetriol triacetate at 24.5°C was re- corresponding mole fraction, $x_2$ , value
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Nothing was specified in the paper.	(1) Not specified.
	(2) Not specified.
	(2) NOU SPECIFIED.
	ESTIMATED ERROR:
	Temp. ±0.5 <sup>°</sup> C (mean of reported range).
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1,2,3-Propanetriol triacetate   (glycerol triacetate); C<sub>9</sub>H<sub>14</sub>O<sub>6</sub>;</pre>	Kraus, K.A.; Raridon, R.J.; Baldwin, W.H.
[102-76-1] (2) Water; H <sub>2</sub> O; [7732-18-5]	J. Am. Chem. Soc. <u>1964</u> , 86, 2571-6.
VARIABLES:	PREPARED BY:
T/K = 298	Z. Maczynska
EXPERIMENTAL VALUES: The solubility of 1,2,3-propanetriol ported to be 7.4 g(1)/100g sln. The calculated by the compiler is 0.0066	triacetate in water at 25 <sup>0</sup> C was re- corresponding mole fraction, <i>x</i> <sub>1</sub> , value
The solubility of water in $1,2,3$ -proported to be $4.60 \text{ g}(2)/100\text{ g} \text{ sln}$ . The value calculated by the compiler is (	panetriol triacetate at $25^{\circ}$ C was re- corresponding mole fraction, $x_2$ , 0.369.
value calculated by the compiler is (	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical methods were used. The mutual solubilities of (1) and (2) were determined by shaking mixtures in stoppered tubes in a constant temperature bath The	(1) Source not specified; commercial product; distilled under vacuum and middle fraction 60-80% collected.
(1)-rich phases were analyzed for water by the use of Karl Fischer titrations. The (2)-rich phases	(2) Not specified.
semimicro adaptation of the stand-	ESTIMATED ERROR:
by back titration of excess alkali is performed on a boiling solution to minimize carbonate error, and in a flask under a reflux condenser to	Soly. ±5 g(1)/100g sln and ±1 g(2)/100g sln (precision).
minimize loss of acetic acid.	

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REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Propanoic acid cyclohexyl		Stephenson, R.; Stuart, J.			
ester (cyclohexyl propionate);		T Chom Eng Data 1986 21			
C <sub>9</sub> H <sub>16</sub> O <sub>2</sub> ; [6222-35-1]		56-70.	<u> 1900</u> , 01,		
(2) Wat	er; H <sub>2</sub> O; [7732-1	8-5]			
VARIABLES	:		PREPARED BY:		
T/K = 27	3 - 364		Z. Maczynska		
EXPERIMEN	TAL VALUES:		I		
Mutual solubility of propanoic acid cyclohexyl ester and water				r and water	
				1or)	
ι/ τ	(2)-rich phase	(1)-rich nhas	$x_1$ (complete $x_1$ (comple	(1)-rich phase	
0	0.109	99.17	0.000126	0.9323	
9.5	0.096	99.29	0.000111	0.9416	
20.2	0.079	99.21	0.000091	0.9354	
30.6	0.073	99.06	0.000084	0.9239	
39.6	0.065	99.18	0.000075	0.9331	
50.0	0.061	99.32	0.000070	0.9439	
60.1	0.073	99.28	0.000084	0.9408	
70.2	0.066	99.06	0.000076	0.9239	
80.2	0.080	98.91	0.000092	0.9127	
90.6	0.075	98.78	0.000086	0.9032	
std. d	ev. 0.001	0.05			
		AUXILIARY	INFORMATION		
METHOD/AP	PARATUS/PROCEDUR	E:	SOURCE AND PURITY C	F MATERIALS:	
mha analu			(1) Gauna wat and	-161-3	
Componen	t (1) was equili	s used. brated	cial sample; purity 99%; used		
with com	ponent (2) at a	given tat Fach	as received.		
layer was	s sampled with a	syringe;	(2) Not specified.		
(1) was (	determined by ad	ding a			
(or some	times propanol)	to the			
organic bv a Gow	layer sample and -Mac thermal con	measuring ductivity	ESTIMATED ERROR:		
gc the (	1)/acetonitrile	peak ratio	Accuracy of method	0.1 wt <sup>9</sup> on logg	
(Chromos) 3390 A r	orb 101 packing ecorder-integrat	and a HP or).	for solubility, se	e above.	
A similar	r procedure but	a higher			
was used	material (e.g. 1 to determine (2	-nexanol) ) in the			
water lag	yer.		REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Pentanedioic acid diethyl ester ( <i>diethyl glutarate</i> ); $C_9H_{16}O_4$ ; [818-38-2] (2) Water; $H_2O$ ; [7732-18-5]	Sobotka, H.; Kahn, J. <i>J. Am. Chem. Soc</i> . <u>1931</u> , 53, 2935-8.	
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of pentanedioic acid diethyl ester in water at 20°C was re- ported to be 0.882 g(1)/100mL(2). The corresponding mass per cent and mole fraction, $x_1$ , values calculated by the compiler are 0.876 g(1)/100g sln and 8.45 x 10 <sup>-4</sup> .		

Density of water  $d_4^{20} = 0.9982$  (ref 1) was used in the calculation.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent droplets.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified (Eastman Kodak Laboratories or synthe- sized); twice-distilled under reduced pressure; d<sup>20</sup> 1.0220, n<sup>20</sup> 1.4242. (2) Distilled. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES: 1. Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, 1973.</pre>		

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COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Acetic acid heptyl ester		Stephenson, R.; Stuart, J.			
( <i>heptyl acetate</i> ); C <sub>9</sub> H <sub>18</sub> O <sub>2</sub> ; [112-06-1]		J. Chem. Eng. Data <u>1986</u> , 31, 56-70.			
(2) Wat	$er: H_0: [7732-1]$	8-51			
UNDING FC		······			
VARIADIES	•		PREFARED DI.		
T/K = 273	3 - 364		Z. Maczynska		
EXPERIMENT	FAL VALUES:		<u></u>		
1	Mutual solubilit	y of acetic a	cid heptyl ester an	d water	
t/°C	g(1)/10	0g sln	$x_1$ (comp:	iler)	
	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase	
0	0.023	99.66	0.000026	0.9709	
9.2	0.018	99.62	0.000020	0.9676	
19.0	0.020	99.55	0.000023	0.9618	
30.8	0.023	99.52	0.000026	0.9593	
40.3	0.021	99.41	0.000024	0.9504	
50.0	0.020	99.41	0.000023	0.9504	
70.2	0.013	99 <b>.</b> 37	0.000022	0.9472	
70.2	0.017	99.35	0.000019	0.9450	
00.4	0.015	99.33	0.000017	0.9440	
	0.019				
std. de	ev. 0.001	0.01			
AUXILIARY INFORMATI			INFORMATION		
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:			
The analy	vtical method wa	s used.	(1) Source not sp	ecified, commer-	
Component	: (1) was equili	brated	cial sample; ]	purity 98%; used	
temperati	ire in a thermos	given stat. Each	as received.		
layer was	s sampled with a	syringe;	(2) Not specified.		
(1) was determined by adding a weighed amount of acetonitrile					
(or sometimes propanol) to the					
by a Gow-	-Mac thermal con	ductivity	ESTIMATED ERROR:		
gc the (1	L)/acetonitrile	peak ratio and a HP	Accuracy of method	1 0.1 wt% or less,	
(Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-boyanol)		for solubility, se	ee above.		
was used to determine (2) in the					
water layer.		REFERENCES:			

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Butanoic acid 3-methyl-1-butyl		Stephenson, R.: Stuart, J.		
ester (isopentyl butyrate);				
c	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub> ; [106-27-4]		56-70.	a <u>1960</u> , 51,
(2) W	ater; H <sub>2</sub> O; [7732-	18-5]		
VARIABL	ES:		PREPARED BY:	<u> </u>
T/K = 2	273 - 364		Z. Maczynska	•
FYDEDTM	ENTAL VALUEC.	<u></u>	<u></u>	<u> </u>
Mutu	al solubility of 1	butanoic acid	3-methyl-1-butyl es	ter and water
t/°C	q(1)/1	 OOq sln	x. (compiler)	
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase
<u> </u>		99 75		0.9784
9.4	0.035	99.75	0.000040	0.9751
19.6	0.022	99.76	0.000025	0.9793
30.9	0.027	99.62	0.000031	0.9676
39.9	0.015	99,59	0.000017	0.9651
49.8	0.037	99.69	0.000042	0.9734
59.7	0.013	99.68	0.000015	0.9726
70.2	0.014	99.61	0.000016	0.9667
80.1	0.024	99.52	0.000027	0.9593
90.7	0.020	99.50	0.000023	0.9577
std.	dev. 0.004	0.01		
	AUXILIARY		INFORMATION	
METHOD / APPARATUS / PROCEDURE :		SOURCE AND PURITY	OF MATERIALS:	
The ana Compone with co tempera	The analytical method was used. Component (1) was equilibrated with component (2) at a given		<ol> <li>Source not specified, commer- cial sample; purity 99%; used as received.</li> </ol>	
layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.		(2) Not specified		
		ESTIMATED ERROR:		
		Accuracy of method 0.1 wt% or less, for solubility, see above.		
		REFERENCES:		
J				
L				

T

COMPONENTS:	EVALUATOR:
<pre>(1) Butanoic acid pentyl ester (pentyl butyrate); C<sub>9</sub>H<sub>18</sub>O<sub>2</sub>; [540-18-1]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2) Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988
CRITICAL EVALUATION:	

CRITICAL EVALUATION:

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

<u>TABLE 1: Quantitative Solubility Studies of the</u> Butanoic acid pentyl ester (1) - Water (2) System			<u>of the</u> System
Reference	T/K	Solubility	Method
Hemptinne (ref 1)	298	(1) in (2)	analytical
Stephenson and Stuart (ref 2)	273-364	mutual	GLC

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. SOLUBILITY OF BUTANOIC ACID PENTYL ESTER (1) IN WATER (2)

All the available data for the solubility of butanoic acid pentyl ester (1) in water (2) are summarized in Table 2. At 298 K, the only temperature where comparison is possible, the data of Hemptinne (ref 1) and Stephenson and Stuart (ref 2) are in only fair agreement. At other temperatures only the data of Stephenson and Stuart (ref 2) are available. Although the solubilities reported by these authors are usually reliable it should be noted that their results for this system are very scattered. Consequently, all the values in Table 2 should be regarded as very Tentative, pending further studies.

(continued next page)

COMPONENTS:	EVALUATOR:		
<ul> <li>(1) Butanoic acid pentyl ester (<i>pentyl butyrate</i>); C<sub>9</sub>H<sub>18</sub>O<sub>2</sub>; [540-18-1]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia		
	December, 1988		
CRITICAL EVALUATION: (continued)			
<u>TABLE 2: Tenta</u> of Butanoic acid penty	<u>tive Solubilities</u> L <u>ester (1) in Water (2)</u>		
 T/K Sol	lubilities		
Reported values <sup>a</sup>	"Best" values <sup>b</sup>		
g(1)/100g sln	$g(1)/100g sln 10^5 x_1$		
273 0.03 <sup>*</sup> (ref 2)	0.03 3		
283 0.03 <sup>*</sup> (ref 2)	0.03 3		
293 0.03 <sup>*</sup> (ref 2)	0.03 3		
298 0.050 (ref 1), 0.03* (ref 2	2) $0.04 \pm 0.01^{c}$ 5		
303 0.03 <sup>*</sup> (ref 2)	0.03 3		
313 0.03 <sup>*</sup> (ref 2)	0.03 3		
323 0.03 <sup>*</sup> (ref 2)	0.03 3		
333 0.03 <sup>*</sup> (ref 2)	0.03 3		
343 0.03 <sup>*</sup> (ref 2)	0.03 3		
353 0.02 <sup>*</sup> (ref 2)	0.02 2		
363 0.02 <sup>*</sup> (ref 2)	0.02 2		
<sup>4</sup> Data in ref 2 very scattered.			
<sup>b</sup> Rounded values of ref 2, except at	: 298 K.		
<sup>c</sup> Average value; $x_1$ has the same (relative) percentage uncertainty as the mass % solubility.			
2. SOLUBILITY OF WATER (2) IN BUTANOIC ACID PENTYL ESTER (1)			
Only the data of Stephenson and Stuart (ref 2) are available for the solubility of water (2) in butanoic acid pentyl ester (1) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental solubilities. It should be noted, however, that whilst the solubilities reported by these authors are generally reliable, their results for this system are very scattered. Further studies are clearly required.			
REFERENCES			
1. Hemptinne, A. Z. Phys. Chem. <u>1894</u> , 13, 561-9.			

2. Stephenson, R.; Stuart, J. J. Chem. Eng. Data 1986, 31, 56-70.

	-
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butanoic acid pentyl ester	Hemptinne, A.
(pentyl butyrate); C <sub>9</sub> H <sub>18</sub> O <sub>2</sub> ;	Z. Phys. Chem. <u>1894</u> , 13, 561-9.
[540-18-1]	
(2) water; H <sub>2</sub> O; [//32-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
to be 0.505 g(1)/L sln.	Y CSTEL IN WOOL OF 25 C Was reported
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The mixture of water with excess ester was heated for some time in a water bath and the ester phase was fil- tered. A sample of known volume was then transferred to a smaller	<ul><li>(1) Not specified.</li><li>(2) Not specified.</li></ul>

flask, heated with the known amount of baryta until complete saponifi-cation was obtained and then ti-trated. No further details were re-ported in the paper. ESTIMATED ERROR:

Not specified.

**REFERENCES:** 

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Butanoic acid pentyl ester   (pentyl butyrate); C<sub>9</sub>H<sub>18</sub>O<sub>2</sub>;   [540-18-1]</pre>	Stephenson, R.; Stuart, J. <i>J. Chem. Eng. Data</i> <u>1986</u> , 31, 56-70.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 273 - 364	Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of butanoic acid pentyl ester and water

t/°C	g(1)/10	0g sln	$x_1$ (comp	iler)
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	0.026	99.54	0.000030	0.9610
9.4	0.034	99.66	0.00039	0.9709
19.2	0.025	99.60	0.000028	0.9659
29.6	0.024	99.65	0.000027	0.9701
40.1	0.030	99.48	0.000034	0.9561
50.0	0.032	99.61	0.000036	0.9667
60.0	0.028	99.56	0.000032	0.9626
70.3	-	99.38	-	0.9480
80.0	0.019	99.52	0.000022	0.9593
90.5	0.025	99.44	0.000028	0.9529

std. dev. 0.002 0.01

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AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer- cial sample; purity 99%; used as received. (2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above. REFERENCES:</pre>		

1	46	
1	40	

COMPONENTS:		ORIGINAL MEASUREME	NTS:	
(1) Formic acid octyl ester		Stephenson, R.; S	tuart, J.	
(octyl formate); C <sub>9</sub> H <sub>18</sub> O <sub>2</sub> ; [112-32-3]			J. Chem. Eng. Dat 56-70.	a <u>1986</u> , 31,
(2) Water; H <sub>2</sub> O; [7732-18-5]				
VARIABLES:			PREPARED BY:	
T/K = 273 - 364			Z. Maczynska	
EXPERIMENTAL VALUES:			I	
Mutual solubility of formic a		ncid octyl ester and	l water	
t/°C	q(1)/10	log sln	$x_1$ (comp	iler)
(:	2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase
0	<u> </u>	99.579		0.96419
9.2	0.078	99.555	0.000089	0.96222
19.0	0.064	99.583	0.000073	0.96452
29.4	0.039	99.572	0.000044	0.96361
39.5	0.040	99.555	0.000045	0.96222
50.0	0.071	99.545	0.000081	0.96140
60.0	0.028	99.522	0.000032	0.95952
70.1	0.044	99.506	0.000050	0.95821
80.2	0.036	99.426	0.000041	0.95174
90.5	0.061	99.461	0.000069	0.95456
std. dev. 0.003 0.003				
		AUXILIARY	INFORMATION	
		)F•	SOURCE AND DURTTY	OF MATERIALS.
The analyti Component (	.cal method wa (1) was equili	s used. brated	(1) Source not sp cial sample;	ecified, commer- purity 99%; used
with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile		as received. (2) Not specified		
organic lay	ver sample and	measuring		
by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol)		Accuracy of metho for solubility, s	d 0.1 wt% or less, ee above.	
water layer	· · · · · · · · · · · · · · · · · · ·	,	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Heptanoic acid ethyl ester</pre>	Sobotka, H.; Kahn, J.
(ethyl heptanoate); C <sub>9</sub> H <sub>18</sub> O <sub>2</sub> ;	<i>J. Am. Chem. Soc.</i> <u>1931</u> , <i>53</i> ,
[106-30-9]	2935-8.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

## EXPERIMENTAL VALUES:

The solubility of heptanoic acid ethyl ester in water at 20°C was reported to be 0.029 g(1)/100mL(2). The corresponding mass per cent and mole fraction,  $x_1$ , values calculated by the compiler are 0.029 g(1)/100g sln and 3.3 x 10<sup>-5</sup>.

Density of water  $d_4^{20} = 0.9982$  (ref 1) was used in the calculation.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica-] tor particles into dark transparent droplets.	<pre>INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Source not specified (Eastman Kodak Laboratories or synthe- sized); twice-distilled under reduced pressure; n<sup>20</sup><sub>D</sub> 1.4137. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES: 1. Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas,</pre>		
	<u>1973</u> .		

COMPONENT	nc •		OPTOTNAL MEASUREME	NITC .
COMPONENT	to.		Depektoin D.I.	muchimen ) N .
(1) Per	itanoic acid 1-bu itvl valerate): C	cyl ester	Serafimov, L.A.	Trorimov, A.N.;
[59	91-68-4]	918-21	Zh. Prikl. Khim.	<u>1978</u> , 51, 1280-2.
(2) Water; H <sub>2</sub> O; [7732-18-5]				
VARTABLES:		DEEDADED BY.		
VARIABLES:		PREPARED DI:		
T/K = 293 - 363			A. Skrzecz	
EXPERIMEN	TAL VALUES:			
Мі	tual solubility	of pentanoic	acid 1-butyl ester	and water
t/°C	x	1	g(1)/100g sl	n (compiler)
	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase
20	0.00002	0.9037	0.02	98.80
30	0.00009	0.8821	0.08	98.50
40	0.00015	0.8751	0.13	98.40
50	0.00021	0.8514	0.18	98.05
60	0.00027	0.8319	0.24	97.75
70	0.00037	0.8163	0.32	97.50
80	0.00039	0.8011	0.34	97.25
90	0.00046	0.7865	0.40	97.00
		AUXILIARY 1	INFORMATION	
METHOD/AF	PARATUS/PROCEDUR	Е:	SOURCE AND PURITY	OF MATERIALS:
The titr constant details	ation method was temperature. No were reported in	used at further the paper.	(1) Source not sp led; without b.p. 185.3 <sup>o</sup> C,	ecified; distil- impurities by glc, $n_{\rm D}^{20}$ 1.412.
			(2) Not specified	
			ESTIMATED ERROR:	
		Not specified		
			Not specified.	
			DEFEDENCES .	
			Kerenced:	

COMPONENT	rs:		ORIGINAL MEASUREME	NTS:
(1) Pro	panoic acid hexy	yl ester	Stephenson, R.; S	tuart, J.
(he	exyl propionate)	; C <sub>9</sub> H <sub>18</sub> O <sub>2</sub> ;	J. Chem. Eng. Dat	a 1986. 3 <i>1</i> .
[24	45-76-3]		56-70.	- <u></u> ,,
(2) Wat	(2) Water; H <sub>2</sub> O; [7732-18-5]			
VARIABLES	3:		PREPARED BY:	<u> </u>
T/K = 273 - 364		Z. Maczynska		
	EXPERIMENTAL VALUES:		j	·
EXPERIMEN	NTAL VALUES: Mutual solubility	of propanoic	acid hevyl ester a	und water
t/°C	g(1)/10	00g sln	$x_1$ (comp	iler)
	(2)-rich phase	(1) -rich phas	se (2)-rich phase	(1)-rich phase
0	0.029	99.61	0.000033	0.9667
9.7	0.022	99.66	0.000025	0.9709
20.0	0.024	99.66	0.000027	0.9709
29.6	0.012	99.55	0.000014	0.9618
39.8	0.012	99.52	0.000014	0.9593
50.0	0.014	99.54	0.000016	0.9610
60.0	0.016	99.50	0.000018	0.9577
70.3	0.018	99.51	0.000020	0.9585
80.3	0.017	99.49	0.000019	0.9569
90.6	0.018	99.17	0.000020	0.9315
std. d	lev. 0.001	0.02		
	· · · · · · · · · · · · · · · · · · ·			
METHOD/AP	PPARATUS/PROCEDUF	<b>ξΕ:</b>	SOURCE AND PURITY	OF MATERIALS:
The anal	ytical method wa	is used.	(1) Source not sp	ecified, commer-
Componen with com	it (1) was equili ponent (2) at a	diven	cial sample; as received.	purity 99%; used
temperat	ure in a thermos	stat. Each	(2) Not croatfied	
(1) was	determined by ad	lding a	(2) Not specified	•
weighed	amount of acetor	itrile to the		
organic	layer sample and	measuring	ESTIMATED ERROR:	
by a Gow	Mac thermal cor 1)/acetonitrile	peak ratio	ESTIMATED ERROR:	
(Chromos	orb 101 packing	and a HP	Accuracy of metho for solubility. s	d 0.1 wt% or less, ee above.
A simila	r procedure but	a higher		
boiling	material (e.g. 1	-hexanol)		
was used water la	yer.	.) In the	REFERENCES:	
L				

à

COMPONENT	omponents:		ORIGINAL MEASUREMENTS:	
<ol> <li>Dibutylphosphinic acid methyl ester (methyl dibutylphosphinate); C<sub>9</sub>H<sub>21</sub>O<sub>2</sub>P; [7163-67-9]</li> <li>Water; H<sub>2</sub>O; [7732-18-5]</li> </ol>		Nikolaev, A.V.; Dyadin, Yu.A.; Yakovlev, I.I.; Durasov, V.B.; Yakovleva, N.I.; Khol'kina, I.D Zh. Fiz. Khim. <u>1966</u> , 40, 221-3.		
ARIABLES	;:		PREPARED BY:	
T/K = 30	r/K = 309 - 464		A. Skrzecz	
Mutual t/°C	g(1)/1	dibutylphosph	inic acid methyl est $x_1$ (comp	er and water iler)
Mutual  t/°C	g(1)/1 (2)-rich phase	dibutylphosph 00g sln (1)-rich pha	inic acid methyl est x <sub>1</sub> (comp se (2)-rich phase	er and water iler) (1)-rich phase
Mutual t/°C  35.5 I	g(1)/1 (2)-rich phase CST 19.83	dibutylphosph 00g sln (1)-rich pha 19.83	inic acid methyl est $x_1$ (complete 	er and water iler) (1)-rich phase 0.02265
Mutual t/°C 35.5 I 36.2	g(1)/1 (2)-rich phase CST 19.83 12.75	dibutylphosph 00g sln (1)-rich pha 19.83	inic acid methyl est x <sub>1</sub> (comp .se (2)-rich phase 0.02265 0.01351	er and water iler) (1)-rich phase 0.02265
Mutual t/°C 35.5 I 36.2 36.6	g(1)/1 (2)-rich phase CST 19.83 12.75	dibutylphosph 00g sln (1)-rich pha 19.83 	$\frac{x_1 \text{ (comp)}}{x_2 \text{ (comp)}}$	er and water iler) (1)-rich phase 0.02265 - 0.04049 0.02100
Mutual t/°C 35.5 I 36.2 36.6 37.0 22.0	g(1)/1 (2)-rich phase CST 19.83 12.75 -	dibutylphosph 00g sln (1)-rich pha 19.83 - 31.05 36.87	inic acid methyl est x <sub>1</sub> (comp (2)-rich phase 0.02265 0.01351 - -	er and water iler) (1)-rich phase 0.02265 - 0.04049 0.05189 0.05260
Mutual t/°C 35.5 I 36.2 36.6 37.0 38.0 40.2	g(1)/1 (2)-rich phase CST 19.83 12.75 - - - - -	dibutylphosph 00g sln (1)-rich pha 19.83 - 31.05 36.87 42.02	inic acid methyl est x <sub>1</sub> (comp: (2)-rich phase 0.02265 0.01351 - - - 0.02743	er and water iler) (1)-rich phase 0.02265 - 0.04049 0.05189 0.06360
Mutual t/°C 35.5 L 36.2 36.6 37.0 38.0 40.2 41.0	g(1)/1 (2)-rich phase CST 19.83 12.75 - - - 7.40	dibutylphosph 00g sln (1)-rich pha 19.83 - 31.05 36.87 42.02 - 46.14	inic acid methyl est x <sub>1</sub> (comp (2)-rich phase 0.02265 0.01351 - - - 0.00743 -	er and water iler) (1)-rich phase 0.02265 - 0.04049 0.05189 0.06360 - 0.07431
Mutual t/°C 35.5 I 36.2 36.6 37.0 38.0 40.2 41.0 47.2	g(1)/1 g(1)/1 (2)-rich phase CST 19.83 12.75 - - - - 7.40 -	dibutylphosph 00g sln (1)-rich pha 19.83 - 31.05 36.87 42.02 - 46.14 52.49	inic acid methyl est x <sub>1</sub> (comp: (2)-rich phase 0.02265 0.01351 - - 0.00743 -	er and water iler) (1)-rich phase 0.02265 - 0.04049 0.05189 0.06360 - 0.07431 0.09382
Mutual t/°C 35.5 I 36.2 36.6 37.0 38.0 40.2 41.0 47.2 50.0	. solubility of g(1)/1 (2)-rich phase CST 19.83 12.75 - - 7.40 - - 4.85	dibutylphosph 00g sln (1)-rich pha 19.83 	inic acid methyl est x <sub>1</sub> (comp: (2)-rich phase 0.02265 0.01351 - - 0.00743 - 0.00743 - 0.00475	er and water iler) (1)-rich phase 0.02265 - 0.04049 0.05189 0.06360 - 0.07431 0.09382 -
Mutual t/°C 35.5 I 36.2 36.6 37.0 38.0 40.2 41.0 47.2 50.0 56.3	g(1)/1 (2)-rich phase CST 19.83 12.75 - - - 7.40 - 4.85 -	dibutylphosph 00g sln (1)-rich pha 19.83 - 31.05 36.87 42.02 - 46.14 52.49 - 57.58	inic acid methyl est x <sub>1</sub> (comp: (2)-rich phase 0.02265 0.01351 - - 0.00743 - 0.00475 -	er and water iler) (1)-rich phase 0.02265 - 0.04049 0.05189 0.06360 - 0.07431 0.09382 - 0.11285
Mutual t/°C 35.5 I 36.2 36.6 37.0 38.0 40.2 41.0 47.2 50.0 56.3 58.0	g(1)/1 g(1)/1 (2)-rich phase CST 19.83 12.75 - - - 7.40 - 4.85 - 3.79	dibutylphosph 00g sln (1)-rich pha 19.83 - 31.05 36.87 42.02 - 46.14 52.49 - 57.58	inic acid methyl est x <sub>1</sub> (comp: (2)-rich phase 0.02265 0.01351 - - 0.000743 - 0.000475 - 0.00368	er and water iler) (1)-rich phase 0.02265 - 0.04049 0.05189 0.06360 - 0.07431 0.09382 - 0.11285 -

(continued next page)

AUXILIARY INFORMATION				
AUXILIARY METHOD/APPARATUS/PROCEDURE: The Alekseev's synthetic method was used. A water or glycerine bath was used for temperature control. Ester hydrolysis was not observed. No further details were reported in the paper.	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Synthesized; distilled 5-6 times under vacuum; $d_4^{25}$ 0.9501, $n_D^{25}$ 1.4441. (2) Not specified. ESTIMATED ERROR: Not specified.			
	REFERENCES:			

OMPONENT	'S:	0	RIGINAL MEASUREME	INTS:
<ol> <li>Dibutylphosphinic acid methyl ester (methyl dibutylphosphinate); C<sub>9</sub>H<sub>21</sub>O<sub>2</sub>P; [7163-67-9]</li> <li>Water; H<sub>2</sub>O; [7732-18-5]</li> </ol>		acid methyl sphinate); <sup>.9</sup> ] 18-5]	Nikolaev, A.V.; D Yakovlev, I.I.; Yakovleva, N.I. Zh. Fiz. Khim. <u>1</u>	yadin, Yu.A.; Durasov, V.B.; ; Khol'kina, I.I <u>966</u> , 40, 221-3.
XPERIMEN Mutual	TAL VALUES: (co solubility of (	ontinued) dibutylphosphini	ic acid methyl est	cer and water
t/°C	g(1)/10	00g sln	x_1 (comp	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
64.0	3.46		0.00335	
68.0	3.29	-	0.00318	-
71.0	-	62.20	-	0.13360
90.5	-	65.14	**	0.14902
120.0	3.29	-	0.00318	-
133 0	-	65.14	-	0.14902
122.0				
150.0	4.85	-	0.00475	-
150.0 155.0	4.85	- 62.20	0.00475 -	- 0.13360
150.0 155.0 171.0	4.85 - -	- 62.20 57.58	0.00475 - -	- 0.13360 0.11285
150.0 155.0 171.0 172.0	4.85 - - 7.40	- 62.20 57.58 -	0.00475 - - 0.00743	- 0.13360 0.11285 -
155.0 155.0 171.0 172.0 181.0	4.85 - 7.40 -	- 62.20 57.58 - 52.49	0.00475 - - 0.00743 -	- 0.13360 0.11285 - 0.09382
155.0 155.0 171.0 172.0 181.0 186.0	4.85 - 7.40 - 12.75	- 62.20 57.58 - 52.49 -	0.00475 - - 0.00743 - 0.01351	- 0.13360 0.11285 - 0.09382 -
155.0 155.0 171.0 172.0 181.0 186.0 190.0	4.85 - 7.40 - 12.75 19.83	- 62.20 57.58 - 52.49 - 42.02	0.00475 - - 0.00743 - 0.01351 0.02265	- 0.13360 0.11285 - 0.09382 - 0.06360

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COMPONENTS: (1) Methylphosphonic acid dibutyl			ORIGINAL MEASUREMEN Nikolaev, A.V.; D	NTS: yadin, Yu.A.;	
est ( <i>di</i>	er butyl methylpho	sphonate);	Yakovlev, I.I.; Durasov, V.B.; Yakovleva, N.I.; Khol'kina, I.D.		
C <sub>9</sub> H <sub>21</sub> O <sub>3</sub> P; [2404-73-1]		Zh. Fiz. Khim. <u>19</u>	<u>967</u> , 41, 1815-7.		
(2) Water; H <sub>2</sub> O; [7732-18-5]					
VARIABLES:			PREPARED BY:		
T/K = 275 - 348			A. Skrzecz		
EXPERIMENTAL VALUES:		<u></u>			
Mutua	l solubility of	methylphospho	onic acid dibutyl es	ter and water	
t/°C	g(1)/1	00g sln	$x_1$ (comp	iler)	
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase	
1.6	_	60.82	-	0.11840	
4.3	3.49	-	0.00312	-	
7.5	3.02	-	0.00269	-	
8.4	-	64.88	-	0.13780	
8.7	2.94	-	0.00261	-	
18.2	-	69.20	-	0.16274	
19.7	2.00	-	0.00176	-	
28.0	-	72.09	-	0.18265	
34.0	1.49	-	0.00131	-	
44.5	-	75.30	-	0.20870	
75.0	-	78.34	-	0.23833	
	<u></u>	· · · · · · · · · · · · · · · · · · ·			
		AUXILIARY	INFORMATION		
METHOD/AP	PARATUS/PROCEDU	RE:	SOURCE AND PURITY	OF MATERIALS:	
The Alek used. No ported i	seev's syntheti further detail n the paper.	c method was s were re-	(1) Synthesized; distilled 5-6 times under vacuum; $d_4^{20}$ 0.9788, $n_D^{20}$ 1.4255.		
			(2) Not specified	•	
			ESTIMATED ERROR:		
			Not specified.		
			REFERENCES:		

COMPONENTS:	EVALUATOR:
<pre>(1) 1,2-Benzenedicarboxylic acid dimethyl ester (dimethyl phthalate); C<sub>10</sub>H<sub>10</sub>O<sub>4</sub>; [131-11-13]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H <sub>2</sub> O; [7732-18-5]	December, 1988

## CRITICAL EVALUATION:

Quantitative solubility data for the 1,2-benzenedicarboxylic acid dimethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

## TABLE 1: Quantitative Solubility Studies of the 1,2-Benzenedicarboxylic acid dimethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Shanley and Greenspan (ref 1)	RT <sup>a</sup>	(2) in (1)	unspecified
Leyder and Boulanger (ref 2)	293	(1) in (2)	GLC, spectrophotometric

<sup>a</sup> RT - room temperature.

As can be seen from Table 1, there are no independent studies for solubilities in either the  $H_2O$ -rich or organic-rich phases and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheets immediately following this Evaluation for the experimental data.

#### REFERENCES

Shanley, E. S.; Greenspan, F. P. Ind. Eng. Chem. <u>1947</u>, 39, 1536-43.
 Leyder, F.; Boulanger, P. Bull. Environ. Contam. Toxicol. <u>1983</u>, 30, 152-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 1,2-Benzenedicarboxylic acid	Shanley, E.S.; Greenspan, F.P.	
dimethyl ester	Ind. Eng. Chem. 1947, 39, 1536-43.	
(dimethyl phthalate);	,,	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
$\pi/K = room temperature$		
EXPERIMENTAL VALUES: The solubility of water in 1,2-benzenedicarboxylic acid dimethyl ester at room temperature was reported to be 1.6 g(2)/100g(1). The corresponding mass per cent and mole fraction, $x_2$ , values calculated by the compiler are 1.6 g(2)/100g sln and 0.15.		
AUXILIARY :	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Not specified.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	-	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) 1,2-Benzenedicarboxylic acid dimethyl ester (<i>dimethyl phthalate</i>); C<sub>10</sub>H<sub>10</sub>O<sub>4</sub>; [131-11-13]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	Leyder, F.; Boulanger, P. Bull. Environ. Contam. Toxicol. <u>1983</u> , 30(2), 152-7.
VARIABLES: T/K = 293	PREPARED BY: A. Skrzecz
FYDERTMENTAL VALUES.	

The solubility of 1,2-benzenedicarboxylic acid dimethyl ester in water at  $20^{\circ}$ C was reported to be 2.21 x  $10^{-2}$  mol(1)/L and 4.290 g(1)/L.

#### AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD/APPARATUS/PROCEDURE: The analytical method as described (1) Fluka; purity>99>% ; used as in the OECD Guidelines for Testing received. of Chemicals (ref 1) was used. Gas (2) Deionized and distilled from chromatography analyses were conducted on a Girdel 3000 FFLE appa-KMnO<sub>4</sub>. ratus with flame-ionization detection. A 4 mm x 180 m stainless steel column packed with 3% OV-1 on 80-100 mesh Chromosorb W-AW-DMCS ESTIMATED ERROR: and helium at a 20mL/min flow rate were used. Samples were fortified Temp. ±1°C. with an internal standard, extracted, and concentrated to 1 mL of hexane solution. "Solvent-flush" and "hot-needle" injection techniques were used. The two methods gave similar results. Peak heights **REFERENCES:** were measured throughout. UV measurements were made by using 1-cm 1. OECD Guidelines for Testing of cells in a Perkin-Elmer model 552 Chemicals, Paris, OECD, <u>1981</u>. uv-Visible spectrophotometer. (methods 101, 105).

COMPONENTS:	EVALUATOR:
(1) Hexanedioic acid dieth (diethyl adipate); C <sub>10</sub> H	yl ester G.T. Hefter, School of Mathematical A <sub>18</sub> 0 <sub>4</sub> ; and Physical Sciences,
[141-28-6]	Murdoch University, Perth, W.A.,
(2) Water; H <sub>2</sub> O; [7732-18-5]	Australia
	December, 1988

CRITICAL EVALUATION:

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

TABLE 1: Quantitative Solubility Studies of the			
<u>Hexanedioic acid</u>	diethyl este	r (1) - Water (	(2) System
Reference	T/K	Solubility	Method
Sobotka and Kahn (ref 1)	293	(1) in (2)	titration
Gross et al. (ref 2)	303	(1) in (2)	interferometric
Stephenson and Stuart (ref 3)	273-363	mutual	GLC

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. SOLUBILITY OF HEXANEDIOIC ACID DIETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of hexanedioic acid diethyl ester (1) in water (2) are summarized in Table 2. At 293 and 303 K, the only temperatures where comparison is possible, the studies of Sobotka and Kahn (ref 1) and Gross et al. (ref 2) respectively, are in only fair agreement with that of Stephenson and Stuart (ref 3). At other temperatures only the data of Stephenson and Stuart (ref 3) are available. Consequently, all data must be considered Tentative pending further studies although it may be noted that the data of Stephenson and Stuart (ref 3) are generally reliable.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexanedioic acid diethyl ester ( <i>diethyl adipate</i> ); C <sub>10</sub> H <sub>18</sub> O <sub>4</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,
[141-28-6]	Murdoch University, Perth, W.A.,
(2) Water: $H_{-}0$ : [7732-18-5]	Australia
	December, 1988

CRITICAL EVALUATION: (continued)

## TABLE 2: Tentative Solubilities of Hexanedioic acid diethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values	a
	g(1)/100g sln	g(1)/100g sln	10 <sup>4</sup> x <sub>1</sub>
273	1.07 (ref 3)	1.0	9
283	0.87 <sup>*</sup> (ref 3)	0.9	8
293	0.422 (ref 1), 0.69 <sup>*</sup> (ref 3)	$0.6 \pm 0.1^{b}$	5
298	0.64 <sup>*</sup> (ref 3)	0.6	5
303	0.424 (ref 2), 0.60 <sup>*</sup> (ref 3)	$0.5 \pm 0.1^{b}$	4
313	0.54 <sup>*</sup> (ref 3)	0.5	4
323	0.51 <sup>*</sup> (ref 3)	0.5	4
333	0.50 <sup>*</sup> (ref 3)	0.5	4
343	0.50 <sup>*</sup> (ref 3)	0.5	4
353	0.51 <sup>*</sup> (ref 3)	0.5	4
363	0.55* (ref 3)	0.6	5

<sup>a</sup> Rounded values of ref 3 unless otherwise indicated.

<sup>b</sup> Average value; x<sub>1</sub> values have the same (relative) percentage uncertainty as the mass % solubilities.

## 2. SOLUBILITY OF WATER (2) IN HEXANEDIOIC ACID DIETHYL ESTER (1)

As the only available data for the solubility of water (2) in hexanedioic acid diethyl ester (1) are those of Stephenson and Stuart (ref 3) no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental solubilities but it may be noted that the data of these authors are generally reliable (but see Part 1. above).

## REFERENCES

1. Sobotka, H.; Kahn, J. J. Am. Chem. Soc. <u>1931</u>, 53, 2935-8.

- Gross, P. M.; Saylor, J. H.; Gorman, M. A. J. Am. Chem. Soc. <u>1953</u>, 55, 650-2.
- 3. Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u>, 31, 56-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Hexanedioic acid diethyl ester	Sobotka, H.; Kahn, J.	
(diethyl adipate); C <sub>10</sub> H <sub>18</sub> O <sub>4</sub> ; [141-28-6]	J. Am. Chem. Soc. <u>1931</u> , 53, 2935-8.	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of hexanedioic acid diethyl ester in water at 20°C was reported to be 0.423 g(1)/100mL(2). The corresponding mass per cent and mole fraction, $x_1$ , values calculated by the compiler are 0.422 g(1)/100g sln and 3.77 x 10 <sup>-4</sup> . Density of water $d_4^{20} = 0.9982$ (ref 1) was used in the calculation.		
AUXILIARY	INFORMATION	
METHOD / APPARATUS / PROCEDURE •	SOURCE AND PURITY OF MATERIALS.	
The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent droplets.	<ul> <li>(1) Source not specified (Eastman Kodak Laboratories or synthesized); twice-distilled under reduced pressure; d<sup>20</sup><sub>4</sub> 1.0086, n<sup>20</sup><sub>D</sub> 1.4278.</li> <li>(2) Distilled.</li> <li>ESTIMATED ERROR: Not specified.</li> <li>REFERENCES:</li> </ul>	
	<ol> <li>Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, <u>1973</u>.</li> </ol>	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ul> <li>(1) Hexanedioic acid diethyl ester (<i>diethyl adipate</i>); C<sub>10</sub>H<sub>18</sub>O<sub>4</sub>; [141-28-6]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	Gross, P.M.; Saylor, J.H.; Gorman, M.A. <i>J. Am. Chem. Soc.</i> <u>1933</u> , 55, 650-2.	
VARIABLES:	PREPARED BY:	
T/K = 303	Z. Maczynska .	
EXPERIMENTAL VALUES: The solubility of hexanedioic acid diethyl ester in water at $30^{\circ}$ C was reported to be 4.26 g(1)/kg(2) and 0.0211 mol(1)/kg(2). The corresponding mass per cent and mole fraction, $x_1$ , values calculated by the compiler are 0.424 g(1)/100g sln and 3.79 x $10^{-4}$ .		

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The saturated solutions of (1) in (2) were prepared in thin-walled cylindrical flask in a large water thermostat. The saturated solutions were analyzed by means of a Zeiss combination liquid and gas inter- ferometer. The procedure has been previously described in detail by Gross and Saylor (ref 1).	<pre>SOURCE AND PURITY OF MATERIALS: (1) Eastman Kodak Co. best grade; distilled; b.p. range 129.0-129.4°C. (2) Distilled. ESTIMATED ERROR: Temp. ±0.02°C. Soly. ±0.5% (from the concordance of duplicate determinations). REFERENCES: 1. Gross, P.M.; Saylor, J.H. J. Am. Chem. Soc. 1931, 53, 1744.</pre>	

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COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Hexanedioic acid diethyl ester		Stephenson, R.; Stuart, J.		
(diethyl adipate); C <sub>10</sub> H <sub>18</sub> O <sub>4</sub> ; [141-28-6]		J. Chem. Eng. Dat 56-70.	a <u>1986</u> , 31,	
(2) Water; H <sub>2</sub> O	; [7732-18-	5]		
VARIABLES:			PREPARED BY:	
T/K = 273 - 363			Z. Maczynska	
EXPERIMENTAL VAL	UES:			
Mutual solubility of hexanedioic acid diethyl ester and water			r and water	
<i>t/°</i> C g(1)/100g sln		x <sub>1</sub> (comp	piler)	
(2)-ri	ch phase (1	)-rich phas	e (2)-rich phase	(l)-rich phase
0 1	.07	98.92	0.00096	0.8908
9.8 1	.26	98.89	0.00113	0.8881
20.5 0	.69	-	0.00062	-
39.5 0	.54	98.05	0.00048	0.8175
50.0 0	.52	97.89	0.00046	0.8051
60.1 0	.50	97.62	0.00045	0.7851
69.7 0	.50	97.56	0.00045	0.7808
80.2 0	.49	97.17	0.00045	0.7536
90.3 0	.56	97.12	0.00050	0.7502
std. dev. 0.01 0.03				
		AUXILIARY	INFORMATION	
METHOD/APPARATUS	/PROCEDURE:		SOURCE AND PURITY	OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.		<ul> <li>(1) Source not sp cial sample; as received.</li> <li>(2) Not specified</li> </ul>	ecified, commer- purity 99%; used	
		ESTIMATED ERROR: Accuracy of metho for solubility, s	d 0.1 wt% or less, ee above.	
		REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 2-ethylhexyl ester	Doolittle, A.K.
(2-ethylhexyl acetate);	Ind. End. Chem. <u>1935</u> , 27, 1169-79.
C <sub>10</sub> H <sub>20</sub> O <sub>2</sub> ; [103-09-3]	
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES:	I
The solubility of acetic acid 2-ethyl	lhexyl ester in water at 20 <sup>0</sup> C was re-
ported to be very slightly soluble.	
The solubility of water in acetic action $\frac{1}{2}$ ported to be 0.39 g(2)/100g sln. The	corresponding mole fraction, x <sub>2</sub>
value calculated by the compiler is (	0.036.
AUXILIARY 1	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commer- cial product; purity 99%, b.p. range 195-203°C, d <sup>20</sup> 0.873.
	$n_{\rm D}^{20}$ 1.4300.
	(2) Not specified.
	LOTIMATED ERROR:
	Not specified.
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ul> <li>(1) Acetic acid octyl ester (octyl acetate); C<sub>10</sub>H<sub>20</sub>O<sub>2</sub>; [112-14-1]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	Carbide and Carbon Chemicals Corporation, Solvent Chart. Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. <u>1941</u> , 33, 1240-8,	
	1513.	
VARIABLES:	PREPARED BY:	
T/K = 296	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid octyl ester in water at 23°C was reported to be less than 0.3 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calculated by the compiler is less than 3 x 10 <sup>-5</sup> . The solubility of water in acetic acid octyl ester at 23°C was reported to be 0.55 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calcu- lated by the compiler is 0.050.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Nothing was specified in the paper.	(1) Not specified.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:			
<ul> <li>(1) Nonanoic acid methyl ester (methyl nonanoate); C<sub>10</sub>H<sub>20</sub>O<sub>2</sub>; [1731-84-6]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	Tewari, Y.B.; Miller, M.M.; Wasik,S.P.; Martire, D.E. <i>J. Chem. Eng. Data</i> <u>1982</u> , 27, 451-4.			
VARIABLES:	PREPARED BY:			
T/K = 298	A. Skrzecz			

EXPERIMENTAL VALUES:

The solubility of nonanoic acid methyl ester in water at  $25^{\circ}C$  was reported to be 1.33 x  $10^{-4}$  mol(1)/L sln. The corresponding value on a mass/volume basis is 0.0229 g(1)/L sln (compiler).

AUXILIARY INFORMATION					
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The aqueous phase was generated by pumping water into the inlet of coated generator column which was thermostated, either by using a minipump or by means of water reservoir using compressed air at 5 psi. The aqueous solution was extracted by the use of a known amount of immiscible with water solution and then analyzed by a gas chromatographic technique.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified; purity >99% by glc. (2) Not specified. ESTIMATED ERROR: Temp. ±0.1°C. Soly. ±1.0%. REFERENCES:				

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COMPO	NENTS:	EVALUATOR:				
(1)	Octanoic acid ethyl ester ( <i>ethyl caprylate</i> ); C <sub>10</sub> H <sub>20</sub> O <sub>2</sub> ; [106-32-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,				
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia December, 1988				

CRITICAL EVALUATION:

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

## TABLE 1: Quantitative Solubility Studies of the Octanoic acid ethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Sobotka and Kahn (ref 1)	293	(1) in (2)	titration
Stephenson and Stuart (ref 2)	283-364	mutual	GLC

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. SOLUBILITY OF OCTANOIC ACID ETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of octanoic acid ethyl ester (1) in water (2) are summarized in Table 2. At 293 K, the only temperature where comparison is possible, the data of Sobotka and Kahn (ref 1) and Stephenson and Stuart (ref 2) disagree by almost an order of magnitude (Table 2). In the absence of other independent studies it is not possible to determine which value is more reliable. At other temperatures, only the data of Stephenson and Stuart (ref 2) are available. Although the solubilities reported by these authors are usually reliable it should be noted that their results for this system are very scattered. For these reasons the data in Table 2 should be regarded as very Tentative pending further studies.

(continued next page)

COMPO	NENTS:	EVALUATOR:				
(1)	Octanoic acid ethyl ester ( <i>ethyl caprylate</i> ); C <sub>10</sub> H <sub>20</sub> O <sub>2</sub> ;	G.T. Hefter, School of Mathematical and Physical Sciences,				
	[106-32-1]	Murdoch University, Perth, W.A.,				
(2)	Water; H <sub>2</sub> O; [7732-18-5]	Australia				
		December, 1988				

CRITICAL EVALUATION: (continued)

#### TABLE 2: Tentative Solubilities of Octanoic acid ethyl ester (1) in Water (2)

T/K	Solubilities							
		Reported values	"Best" values	a				
		g(1)/100g sln	g(1)/100g sln	10 <sup>5</sup> x <sub>1</sub>				
283	0.05*	(ref 2)	0.05	5				
293	0.007	(ref 1), 0.05 (ref 2)	0.05	5				
298	0.04*	(ref 2)	0.04	4				
303	0.04*	(ref 2)	0.04	4				
313	0.04*	(ref 2)	0.04	4				
323	0.04*	(ref 2)	0.04	4				
333	0.04*	(ref 2)	0.04	4				
343	0.04*	(ref 2)	0.04	4				
353	0.04*	(ref 2)	0.04	4				
363	0.04*	(ref 2)	0.04	4				

<sup>a</sup> Rounded values of ref 2, but see text.

## 2. SOLUBILITY OF WATER (2) IN OCTANOIC ACID ETHYL ESTER (1)

As the only available data for the solubility of water (2) in octanoic acid ethyl ester (1) are those of Stephenson and Stuart (ref 2) no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental solubilities. However, it may be noted that the solubilities reported by these authors are generally reliable although the values reported for this particular system are rather scattered (see also Part 1. above).

## REFERENCES

1.	Sobotka,	н.;	Kahn,	J.	J.	Am.	Chem.	Soc.	<u>1931</u> ,	53,	2935-8	3.
2.	Stephenso	n, R	.; st	uart,	J	. ј.	. Chem.	. Eng.	Data	<u>1986</u>	5, 31,	56-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:					
(1) Octanoic acid ethyl ester	Sobotka, H.; Kahn, J.					
$(ethyi caprylate); C_{10}H_{20}O_2;$ [106-32-1]	J. Am. Chem. Soc. <u>1931</u> , 53, 2935-8.					
(2) Water; H <sub>2</sub> O; [7732-18-5]						
VARIABLES:	PREPARED BY:					
T/K = 293	A. Skrzecz					
EXPERIMENTAL VALUES: The solubility of octanoic acid ethyl ester in water at 20°C was reported to be 0.007 g(1)/100mL(2). The corresponding mass per cent and mole frac- tion, $x_1$ , values calculated by the compiler are 0.007 g(1)/100g sln and 7 x 10 <sup>-6</sup> .						
Density of water $d_4^{20} = 0.9982$ (ref 1)	was used in the calculation.					
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:					
The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent	<ul> <li>(1) Source not specified (Eastman Kodak Laboratories or synthesized); twice-distilled under reduced pressure; d<sup>20</sup><sub>4</sub> 0.8674, n<sup>20</sup><sub>D</sub> 1.4197.</li> <li>(2) Distilled.</li> <li>ESTIMATED ERROR: Not specified.</li> </ul>					
aroproop.	REFERENCES:					
	<ol> <li>Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, <u>1973</u>.</li> </ol>					
COMPONENT	'S:		ORIGINAL MEASUREME	NTS:		
---	--	----------------	-------------------------------------	---------------------------------------	--	
(1) Octopoid adid athul octop			Cherkensen D. Stuert I			
(i) Octanoic acid ethyl ester (ethyl caprylate): CioHooOo:			Stephenson, R.; Stuart, J.			
[106-32-1]			J. Chem. Eng. Dat 56-70.	a <u>1986</u> , 31,		
(2) Wat	(2) Water; H <sub>2</sub> O; [7732-18-5]					
VARIABLES	:		PREPARED BY:	, , , , , , , , , , , , , , , , , , ,		
T/K = 27	3 - 364		Z. Maczynska	•		
EXPERIMEN	EXPERIMENTAL VALUES:		I			
	Mutual solubili	ty of octanoid	c acid ethyl ester a	nd water		
t/°C	$t/^{\circ}C$ $\alpha(1)/100\alpha$ sln		x. (compiler)			
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase		
0		99.18	<u> </u>	0.9267		
9.5	0.054	98.85	0.000056	0.8999		
19.6	0.051	99.10	0.000053	0.9201		
30.6	0.038	99.55	0.000040	0.9585		
39.5	-	99.61	-	0.9639		
50.0	0.037	99.35	0.000039	0.9411		
60.1	0.044	99.49	0.000046	0.9533		
70.2	0.040	99.57	0.000042	0.9603		
80.0	0.042	99.59	0.000044	0.9621		
90.6	-	99.61		0.9639		
std. de	ev. 0.003	0.01				
· · · · · · · · · · · · · · · · · · ·		AUXILIARY J				
METHOD/API	PARATUS/PROCEDUF	E:	SOURCE AND PURITY OF MATERIALS:			
The analy	vtical method wa	is used.	(1) Source not specified, commer-			
with comp	c (1) was equili ponent (2) at a	given	as received.	purity 99%; used		
temperati	ure in a thermos	tat. Each	(2) Net englished			
(1) was o	determined by ad	lding a	(2) Not specified.			
weighed a	amount of acetor times propanol)	to the				
organic 1	layer sample and	l measuring	ESTIMATED ERROR:			
gc the (1	1)/acetonitrile	peak ratio	Accuracy of mothed 0.1 with an loss			
(Chromoso 3390 A re	orb 101 packing ecorder-integrat	and a HP	for solubility, so	ee above.		
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the						
water lay	water layer.		REFERENCES:			

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COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Propanoic acid, 2-methyl-,		Stephenson, R.; Stuart, J.			
hexyl ester (hexyl isobutyrate);		J. Chem. Eng. Data 1986. 31.			
		56-70.			
C <sub>10</sub>	<sub>0</sub> H <sub>20</sub> O <sub>2</sub> ; [2349-07-	/]			
(2) Wa	ter; H <sub>2</sub> O; [7732-1	18-5]			
WEDTED		<u> </u>			
VARIABLE	5:		PR	EPARED BY:	
T/K = 2	73 - 364		Z	. Maczynska	
EXPERIME	NTAL VALUES:				
Mutua	al solubility of	2-methylpropa	noi	c acid hexyl est	er and water
t/°C	g(1)/10	)0g sln		$x_1$ (comp	iler)
	(2)-rich phase	(1)-rich phas	е	(2)-rich phase	(1)-rich phase
			-		
0	0.0116	99.50		0.0000121	0.9541
9.4	0.0081	99.69		0.0000084	0.9711
19.5	0.0038	99.63		0.0000040	0.9657
29.7	-	99.74		-	0.9757
39.5	0.0032	-		0.000033	-
50.0	0.0076	99.56		0.0000079	0.9594
59.8	0.0081	-		0.000085	-
70.1	-	99.60		-	0.9630
80.0	0.0040	99.59		0.000042	0.9621
90.6	0.0087	99.58		0.0000091	0.9612
std. d	dev. 0.0005	0.02		· · · · · · · · · · · · · · · · · · ·	and an and a second
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<u> </u>		AUXTLTARY	NEC	PMATTON	
<u> </u>	· · · · · · · · · · · · · · · · · · ·				
METHOD/AI	PPARATUS/PROCEDUP	<b>ξΕ:</b>	SOURCE AND PURITY OF MATERIALS:		
The anal	lytical method wa	is used.	(	1) Source not sp	ecified, commer-
with cor	mponent (2) at a	given	<ul><li>(2) Not specified.</li></ul>		pulley 90%, used
temperat	ture in a thermos	stat. Each			
(1) was	as sampled with a determined by ad	ding a			•
weighed	amount of acetor	itrile			
(or some organic	etimes propanol) laver sample and	to the I measuring			
by a Gov	by a Gow-Mac thermal conductivity		ESTIMATED ERROR:		
gc the ( (Chromos	(1)/acetonitrile	peak ratio	Accuracy of method 0.1 wt% or less		d 0.1 wt% or less,
3390 A 1	recorder-integrat	cor).	f	or solubility, s	ee above.
A simila	ar procedure but	a higher			
was used	d to determine (2	) in the			·····
water la	water layer.		RE	FERENCES:	

COMPONENTS:	EVALUATOR:	
<pre>(1) Acetic acid 2-(2-butoxyethoxy)ethyl ester (2-(2-butoxyethoxy)ethyl acetate); C<sub>10</sub>H<sub>20</sub>O<sub>4</sub>; [124-17-4]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia	
(2) Water; H <sub>2</sub> O; [7732-18-5]	December, 1988	

## CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid 2-(2-butoxyethoxy)ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>TABLE 1: Quantitative Solubility Studies of the</u> Acetic acid 2-(2-butoxyethoxy)ethyl ester (1) - Water (2) System				
Reference	T/K	Solubility	Method	
Doolittle (ref 1)	293	mutual	unspecified	
Othmer et al. (ref 2)	297	mutual	unspecified	

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. They are also summarized in Tables 2 and 3 below.

As there have been only two independent studies at slightly different temperatures, Critical Evaluation is difficult. If the temperature difference is assumed to be negligible (ester-water mutual solubilities do not generally vary dramatically *ca*. 295 K) then the data for the  $H_2O$ -rich phase are in poor agreement whilst the ester-rich phase values are in good agreement. The latter may be regarded as Tentative.

	TABLE 2: Reported Solubilities of Acetic acid 2-(2-butoxyethoxy)ethyl ester (1) in Wat	er (2)
T/K	Reported Solubilities	
	g(1)/100g sln	10 <sup>3</sup> x <sub>1</sub>
293	1.6 (ref 1)	1.4
297	6.5 (ref 2)	6.1

(continued next page)

COMPONENTS:	EVALUATOR:	
<pre>(1) Acetic acid 2-(2-butoxyethoxy)ethyl ester (2-(2-butoxyethoxy)ethyl acetate); C<sub>10</sub>H<sub>20</sub>O<sub>4</sub>; [124-17-4]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia	
(2) Water; H <sub>2</sub> O; [7732-18-5]	December, 1988	

CRITICAL EVALUATION: (continued)

### TABLE 3: Tentative Solubilities of Water (2) in Acetic acid 2-(2-butoxyethoxy)ethyl ester (1)

T/K		Tentative Solubilities	
	g(2)/100g sln		<i>x</i> <sub>2</sub>
293	3.4 (ref 1)		0.29
297	3.7 (ref 2)		0.30

#### REFERENCES

- 1. Doolittle, A. K. Ind. Eng. Chem. <u>1935</u>, 27, 1169-79.
- Othmer, D. F.; White, R. E.; Trueger, E. Ind. Eng. Chem. <u>1941</u>, 33, 1240-8; *ibid.* 1513; see also Carbide and Carbon Chemical Corporation, Solvent Chart, before 1941.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid	Doolittle, A.K.
2-(2-butoxyethoxy)ethyl ester	Ind. End. Chem. <u>1935</u> , 27, 1169-79.
(2 - (2 - bitoxy) = thory) = thy f	
(2) Water: $H \cap [7732-18-5]$	
(2) Water, n <sub>2</sub> 0, [7732-18-5]	
VARIABLES:	PREPARED BY: .
T/K = 293	A. Skrzecz
The solubility of acetic acid 2-(2-bu 20°C was reported to be 1.6 g(1)/100g tion, $x_1$ , value calculated by the com The solubility of water in acetic aci 20°C was reported to be 3.4 g(2)/100g tion, $x_2$ , value calculated by the com	ntoxyethoxy)ethyl ester in water at g sln. The corresponding mole frac- mpiler is 0.0014. id 2-(2-butoxyethoxy)ethyl ester at g sln. The corresponding mole frac- mpiler is 0.29.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified	(1) Source not specified common-
The method was not specified.	(i) Source not specified, commer- cial product; purity 99%, b.p. range 236-249°C, $d_4^{20}$ 0.987.
	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul><li>(1) Acetic acid</li><li>2-(2-butoxyethoxy)ethyl ester</li></ul>	Carbide and Carbon Chemicals Corporation, Solvent Chart.
(2-(2-butoxyethoxy)ethyl acetate); C <sub>10</sub> H <sub>20</sub> O <sub>4</sub> ; [124-17-4]	Othmer, D.F.; White, R.E.; Trueger, E.
(2) Water; H <sub>2</sub> O; [7732-18-5]	Ind. Eng. Chem. <u>1941</u> , 33, 1240-8, 1513.
VARIABLES:	PREPARED BY:
T/K = 297	A. Skrzecz
The solubility of acetic acid 2-(2-bu 23.5°C was reported to be 6.5 g(1)/10 fraction, $x_1$ , value calculated by the The solubility of water in acetic aci 23.5°C was reported to be 3.7 g(2)/10 fraction, $x_2$ , value calculated by the	atoxyethoxy)ethyl ester in water at 10g sln. The corresponding mole 2 compiler is 0.00609. 2d 2-(2-butoxyethoxy)ethyl ester at 10g sln. The corresponding mole 2 compiler is 0.303.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Nothing was specified in the namer	(1) Not specified.
	(2) Not specified
	(2) NOU SPECIFICU.
	ESTIMATED ERROR:
	Temp. ±0.5 <sup>o</sup> C (mean of reported
	range).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Dibutylphosphinic acid eth	Yl Nikolaev, A.V.; Dyadin, Yu.A.;
ester	Yakovlev, I.I.; Durasov, V.B.;
(ethyl dibutylphosphinate)	, i i i i i i i i i i i i i i i i i i i
C <sub>10</sub> H <sub>23</sub> O <sub>2</sub> P; [7100-92-7]	Zh. Fiz. Khim. <u>1966</u> , 40, 221-3.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 287 - 599	A. Skrzecz
EXPERIMENTAL VALUES.	
Mutual solubility of dibutyl	phosphinic acid ethyl ester and water
t/°C g(1)/100g sln	x <sub>1</sub> (compiler)
(2)-rich phase (1)-ric	h phase (2)-rich phase (1)-rich phase
14.0 LCST 23.36 23.3	6 0.02593 0.02593
	7 – 0.04411
	0.00960 -
	4 - 0.07172
	7 - 0.00000
25.4 4.43 -	0.00351 -
41 0 2.44 -	0.00218 -
52.0 2.02 -	0.00180 -
	(continued next page)
AUXTI	TARY INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The Alekseev's synthetic method	was (1) Synthesized; distilled 5-6
used. A water or glycerine bath used for temperature control. E:	was times under vacuum; $d_4^{20}$ 0.9394, ster $n_0^{20}$ 1.4420.
hydrolysis was not observed. No	(2) Not aposified
the paper.	(2) Not specified.
	ESTIMATED ERROR.
	Not specified.
	REFERENCES:

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COMPONENTS:			ORIGINAL MEASUREMENTS:	
<ul> <li>(1) Dibutylphosphinic acid ethyl ester         <ul> <li>(ethyl dibutylphosphinate);</li> <li>C<sub>10</sub>H<sub>23</sub>O<sub>2</sub>P; [7100-92-7]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul> </li> </ul>		ORIGINAL MEASUREMENTS: Nikolaev, A.V.; Dyadin, Yu.A.; Yakovlev, I.I.; Durasov, V.B.; Yakovleva, N.I.; Khol'kina, I.D. Zh. Fiz. Khim. <u>1966</u> , 40, 221-3.		
EXPERIMEN Mutua	NTAL VALUES: (cc al solubility of	ontinued) dibutylphosph	inic acid ethyl est	er and water
t/°C	g(1)/10	0g sln	$x_1$ (compiler)	
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase
54.8	_	70.28		0.17118
58.0	1.79	-	0.00159	-
89.0	-	74.91	-	0.20683
127.0	1.79	-	0.00159	-
159.0	2.44	-	0.00218	-
168.0	-	70.28	-	0.17118
189.0	4.43		0.00403	-
211.0	-	58.65	-	0.11023
216.0	9.99	-	0.00960	-
217.0	-	53.17	-	0.09022
223.0	-	46.94	-	0.07172
225.0		34.57	-	0.04411
226.0 L	JCST 23.36	23.36	0.02593	0.02593

COMPONENT	'S:		ORIGINAL MEASUREME	NTS:	
(1) Dipropylphosphinic acid butyl		Nikolaev, A.V.; Dyadin, Yu.A.;			
ester		Yakovlev, I.I.; Durasov, V.B.;			
(butyl dipropylphosphinate);		Yakovieva, N.I.	; knoi kina, i.D.		
c <sub>10</sub>	H <sub>23</sub> O <sub>2</sub> P; [16984-:	10-4]	Zh. Fiz. Khim. <u>1</u>	<u>967, 41, 1815-7.</u>	
(2) Wat	er; H <sub>2</sub> O; [7732-	18-5]			
VARIABLES	:		PREPARED BY:		
T/K = 27	3 - 448		A. Skrzecz		
EXPERIMEN	TAL VALUES:		L	· · · · · · · · · · · · · · · · · · ·	
Mutual	solubility of	dipropylphospl	ninic acid butyl est	er and water	
t/°C	g(1)/1	.00g sln	$x_1$ (comp	iler)	
	(2)-rich phase	e (1)-rich phas	se (2)-rich phase	(1)-rich phase	
0.0	3.35	13.15	0.003"	0.013	
0.3	-	14.36	-	0.01443	
2.4	5.12	15 76	0.002805	-	
1 2	_	16 62	_	0.01711	
4.2 5.9	2 57	10.02	0 002299	-	
5.8 7 /	2.57	19 70	-	0 02098	
/.4 0 2	_	19.70	_	0.02098	
13.6	-	30 08	-	0.02130	
14.2	1.88	-	0.001671	-	
	2100				
a Exp	erimental value	•			
b Cal	culated by the	compiler.	(cont	cinued next page)	
		AUXILIARY	INFORMATION		
METHOD/AP	PARATUS/PROCEDU	IRE:	SOURCE AND PURITY OF MATERIALS:		
The Alek	seev's syntheti	c method was	(1) Synthesized; distilled 5-6		
used. No	further detail	s were re-	times under vacuum; $d^{20}$ 0 9372 $p^{20}$ 1 4420		
por ceu r	n ene paper.			1111201	
			(2) Not specified	•	
			ESTIMATED ERROR:		
		Not specified.			
		REFERENCES:			
		REFERENCED.			
_					

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1)	Dipropylphosphinic acid butyl ester ( <i>butyl dipropylphosphinate</i> ); C <sub>10</sub> H <sub>23</sub> O <sub>2</sub> P; [16984-10-4]	Nikolaev, A.V.; Dyadin, Yu.A.; Yakovlev, I.I.; Durasov, V.B.; Yakovleva, N.I.; Khol'kina, I.D. Zh. Fiz. Khim. <u>1967</u> , 41, 1815-7.
(2)	Water; H <sub>2</sub> O; [7732-18-5]	
EXPERIMENTAL VALUES: (continued) Mutual solubility of dipropylphosphinic acid butyl ester and water		

t/°c	g(1)/100g sln		x <sub>1</sub> (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
17.2	1.69	_	0.001499	
18.1	-	39.70	-	0.05438
20.8	1.56	-	0.001382	-
23.9	-	49.44	-	0.07869
33.8	1.04	-	0.000917	-
34.0	-	59.62	-	0.11423
53.0	0.651	-	0.000572	-
57.0	-	69.98	-	0.16916
60.7	-	70.76	-	0.17448
89.8	-	74.49	-	0.20321
139.0	-	74.49	-	0.20321
175.0	-	70.76	-	0.17448

COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Ethylphosphonic acid dibutyl ester			Nikolaev, A.V.; Dyadin, Yu.A.; Yakovlev, I.I.; Durasov, V.B.; Yakovleva, N.I.; Khol'kina, I.D.		
					C10
(2) Wat	23 3 7 =	19-51			
(2) Wat	er, n <sub>2</sub> 0, [//32-	10-5]			
VARIABLES	:		PREPARED BY:	•	
T/K = 27	8 - 346		A. Skrzecz		
EXPERIMEN	TAL VALUES:				
Mutua	l solubility of	ethylphospho	nic acid dibutyl este	er and water	
t/°C	g(1)/1	00g sln	$x_1$ (compi	ler)	
-	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase	
5.2	-	73.28		0.1819	
8.6	1.51	-	0.001241	-	
9.8	-	74.87	-	0.1945	
16.2	-	77.06	-	0.2140	
19.5	1.02	-	0.000835	-	
29.5	-	79.94	-	0.2441	
34.5	0.703	-	0.000574	-	
44.4	-	83.31	-	0.2880	
53.0	0.504	-	0.000410	-	
73.0	-	84.62	-	0.3084	
		AUXILIARY	INFORMATION		
ETHOD/AP	PARATUS/PROCEDU	RE:	SOURCE AND PURITY O	F MATERIALS:	
The Alekseev's synthetic method was used. No further details were re- ported in the paper.		(1) Synthesized; d $times$ under va $d_4^{20}$ 0.9658, $n_{\rm D}^{20}$	istilled 5-6 cuum; 1.4290.		
			(2) Not specified.		
			ESTIMATED ERROR.		
			Not chooified		
			Not specified.		
			REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptanedioic acid diethyl	Sobotka, H.; Kahn, J.
ester (diethyl heptanedioate); C <sub>11</sub> H <sub>20</sub> O <sub>4</sub> ; [2050-20-6]	J. Am. Chem. Soc. <u>1931</u> , 53, 2935-8.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of heptanedioic acid of reported to be 0.199 g(1)/100mL(2). The mole fraction, $x_1$ , values calculated sln and 1.66 x 10 <sup>-4</sup> . Density of water $d_4^{20} = 0.9982$ (ref 1)	diethyl ester in water at 20°C was The corresponding mass per cent and by the compiler are 0.199 g(1)/100g was used in the calculation.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent droplets.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified (Eastman Kodak Laboratories or synthe- sized); twice-distilled under reduced pressure; d<sup>20</sup> 0.9945, n<sup>20</sup> 1.4303. (2) Distilled.  ESTIMATED ERROR: Not specified.  REFERENCES: 1. Selected Values of Properties of</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid isononyl ester   (isononyl acetate); C<sub>11</sub>H<sub>22</sub>O<sub>2</sub>;   [40379-24-6]</pre>	Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES: T/K = 273 - 364	PREPARED BY: Z. Maczynska

EXPERIMENTAL VALUES:

.

Mutual solubility of acetic acid isononyl ester and water

t/°C	g(1)/10	0g sln	$x_1$ (comp	iler)
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	0.018	99.666	0.000017	0.96651
9.2	0.023	99.687	0.000022	0.96855
19.4	0.020	99.708	0.000019	0.97061
29.6	0.018	99.628	0.000017	0.96282
39.8	0.021	99.608	0.000020	0.96089
49.8	0.021	99.629	0.000020	0.96292
60.3	0.013	99.631	0.000012	0.96311
70.2	0.018	99.613	0.000017	0.96138
80.3	0.026	99.637	0.000025	0.96369
90.5	0.021	99.598	0.000020	0.95993

std.	dev.	0.002	0.003
	~~~	0.000	0.000

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.	<ul> <li>(1) Source not specified, commer- cial sample; purity 98%; used as received.</li> <li>(2) Not specified.</li> </ul>	
	ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Decanoic acid methyl ester (methyl decanoate); C<sub>11</sub>H<sub>22</sub>O<sub>2</sub>; [110-42-9]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	Tewari, Y.B.; Miller, M.M.; Wasik,S.P.; Martire, D.E. <i>J. Chem. Eng. Data</i> <u>1982</u> , 27, 451-4.
VARTABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of decanoic acid methy to be 2.05 x 10 <sup>-5</sup> mol(1)/L sln. The c basis is 0.00382 g(1)/L sln (compiler	yl ester in water at 25°C was reported corresponding value on mass/volume c).
AUXILIARY	INFORMATION
	SOURCE AND DURTEY OF MATERIALS.
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of a water reservoir using compressed air at 5 psi. The aqueous solution was extracted by the use of a known amount of immiscible-with-water solution and then analyzed by a gas chromatographic technique.	<pre>(1) Source not specified; purity &gt;99% by glc. (2) Not specified. ESTIMATED ERROR: Temp. ±0.1°C. Soly. ±1.0%.</pre>
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) Nonanoic acid ethyl ester (<i>ethyl nonanoate</i>); C<sub>11</sub>H<sub>22</sub>O<sub>2</sub>; [123-29-5]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	Sobotka, H.; Kahn, J. <i>J. Am. Chem. Soc</i> . <u>1931</u> , 53, 2935-8.
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

## EXPERIMENTAL VALUES:

The solubility of Nonanoic acid ethyl ester in water at  $20^{\circ}C$  was reported to be 0.003 g(1)/100mL(2). The corresponding mass per cent and mole fraction,  $x_1$ , values calculated by the compiler are 0.003 g(1)/100g sln and 3 x  $10^{-6}$ .

Density of water  $d_4^{20} = 0.9982$  (ref 1) was used in the calculation.

AUXILIARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE: The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent droplets.	<pre>INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Source not specified (Eastman Kodak Laboratories or synthe- sized); twice-distilled under reduced pressure; n<sup>20</sup> 1.4223. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES:</pre>
	<ol> <li>Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, <u>1973</u>.</li> </ol>

<pre>COMPONENTS: (1) Dibutylphosphinic acid propyl     ester     (propyl dibutylphosphinate);     C<sub>11</sub>H<sub>25</sub>O<sub>2</sub>P; [7100-93-8] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Nikolaev, A.V.; Dyadin, Yu.A.; Yakovlev, I.I.; Durasov, V.B.; Yakovleva, N.I.; Khol'kina, I.D. Zh. Fiz. Khim. <u>1966</u> , 40, 221-3.	
VARIABLES: T/K = 279 - 516	PREPARED BY: A. Skrzecz	
EXPERIMENTAL VALUES: Mutual solubility of dibutylphosphinic acid propyl ester and water		

t/°C	g(1)/100g sln		x <sub>1</sub> (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
6.1		65.22		0.13296
10.0	3.01	-	0.00253	-
13.7	-	69.63	-	0.15789
15.2	-	70.48	-	0.16336
20.5	2.01	-	0.00167	-
27.5	-	74.76	-	0.19499
29.0	1.50	-	0.00124	-
29.8	-	75.31	-	0.19964
41.0	1.01	-	0.00083	-
64.0	0.75	-	0.00062	-
66.5	-	80.58	-	0.25336
143.0	-	80.58	-	0.25336

(continued next page)

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The Alekseev's synthetic method was used. A water or glycerine bath was used for temperature control. No further details were reported in the paper.	<ul> <li>(1) Synthesized; distilled 5-6 times under vacuum; d<sup>20</sup><sub>4</sub> 0.9298, n<sup>20</sup><sub>D</sub> 1.4439.</li> <li>(2) Not specified.</li> </ul>		
	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES:		

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1)	Dibutylphosphinic acid propyl ester (propyl dibutylphosphinate); C <sub>11</sub> H <sub>25</sub> O <sub>2</sub> P; [7100-93-8]	Nikolaev, A.V.; Dyadin, Yu.A.; Yakovlev, I.I.; Durasov, V.B.; Yakovleva, N.I.; Khol'kina, I.D. Zh. Fiz. Khim. <u>1966</u> , 40, 221-3.	
(2)	Water; H <sub>2</sub> O; [7732-18-5]		

EXPERIMENTAL VALUES: (continued)

Mutual solubility of dibutylphosphinic acid propyl ester and water

t/°C	g(1)/100g sln		x <sub>1</sub> (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
176.0	1.41		0.00117	<u> </u>
189.0	-	75.31	-	0.19964
197.0	2.24	-	0.00187	-
208.0	-	70.48	-	0.16336
217.0	4.05	-	0.00344	-
221.0	-	65.22	-	0.13296
230.0	6.86	-	0.00599	-
242.0	17.09	50.32	0.01658	0.07650
243.0 UC	ST 35.08	35.08	0.04232	0.04232

The ester hydrolysis began at temperature 150-170°C.

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COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) Propyipnosphonic acid dibutyi ester			Nikolaev, A.V.; Dy Yakovlev, I.I.; Yakovleva, N.I.;	adin, Yu.A.; Durasov, V.B.; Khol'kina. I.D.	
(dibutyl propylphosphonate);		7h Big Khim 1067 41 1915-7			
	12503F, [4020-12	_0]	211. F12. Mitm. <u>19</u>	<u>07</u> , 41, 1013-7.	
(2) Wat	er; H <sub>2</sub> O; [7732-]	L8-5]			
VARIABLES	:		PREPARED BY:		
T/K = 27	4 - 316		A. Skrzecz		
EXPERIMEN	TAL VALUES:				
Mutua	l solubility of	propylphospho	onic acid dibutyl est	er and water	
t/°c	g(1)/10		x <sub>1</sub> (compi	ler)	
	(2)-rich phase	(1)-rich phas	se (2)-rich phase (	1)-rich phase	
1.2		81.62		0.2529	
9.5	-	83.43	-	0.2774	
11.5	0.596	-	$4.569 \times 10^{-4}$	-	
15.7	0.446	-	$3.414 \times 10^{-4}$	-	
19.4	0.386	-	$2.953 \times 10^{-4}$	-	
22.4	-	85.38	-	0.3081	
23.8	0.324	-	$2.478 \times 10^{-4}$	-	
33.0	-	86.36	-	0.3256	
34.5	0.230	-	$1.757 \times 10^{-4}$	-	
43.0	-	87.06	-	0.3390	
		AUXILIARI			
METHOD/AP	PARATUS/PROCEDU	RE:	SOURCE AND PURITY OF MATERIALS:		
The Alekseev's synthetic method was used. No further details were re- ported in the paper.		(1) Synthesized; distilled 5-6 times under vacuum; $d_4^{20}$ 0.9569, $n_D^{20}$ 1.4309.			
		(2) Not specified.			
			} 		
		ESTIMATED ERROR:			
			Not specified.		
			REFERENCES:		

Γ	1
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Benzenedicarboxylic acid	Shanley, E.S.; Greenspan, F.P.
(diethyl phthalate):	Ind. Eng. Chem. <u>1947</u> , 39, 1536-43.
$C_{12}H_{14}O_{4}$ ; [84-66-2]	
(2) Water: $H \cap [7732-19-5]$	
$(2)$ water, $n_20$ , $[7732-10-5]$	
VARIABLES:	PREPARED BY:
T/K = room temperature	A. Skrzecz
The solubility of water in 1,2-benzer room temperature was reported to be : mass per cent and mole fraction, $x_2$ , 0.99 g(2)/100g sln and 0.11.	hedicarboxylic acid diethyl ester at 1.0 g(2)/100g(1). The corresponding values calculated by the compiler are
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified. No	(1) Not specified.
the paper.	(2) Not specified.
	ESTIMATED ERROR:
	Not googified
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Benzenedicarboxylic acid	Leyder, F.; Boulanger, P.
diethyl ester	Bull. Environ. Contam. Toxicol.
$C_{12}H_{14}O_4$ ; [84-66-2]	<u>1983,</u> 30(2), 152-7.
(2) Water; $H_{2}0$ ; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
FYDERTMENTAL VALUES.	
The solubility of 1,2-benzenedicarbox	wylic acid diethyl ester in water at
20°C was reported to be 4.18 x $10^{-3}$ m	ol(1)/L and 0.928 g(1)/L.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method as described	(1) Merck: purity 99% : used as
in the OECD Guidelines for Testing	received.
chromatography analyses were con-	(2) Deionized and distilled from
aucted on a Girdel 3000 FFLE appa- ratus with flame-ionization detec-	KMnO <sub>4</sub> .
tion. A 4 mm x 180 m stainless steel column packed with 3% OV-1 on	
80-100 mesh Chromosorb W-AW-DMCS and helium at a 20mL/min flow rate	ESTIMATED ERROR:
were used. Samples were fortified	Temp. ±1°C.
ed, and concentrated to 1 mL of	-
and "hot needle" injection tech-	
niques were used. The two methods gave similar results. Peak heights	REFERENCES:
were measured throughout. UV meas- urements were made by using 1-cm	1 OFOD Cuidelines for mostive - f
cells in a Perkin-Elmer model 552	Chemicals, Paris, OECD, <u>1981</u> .
at the speer opin conduct.	(methods 101, 105).

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COMPONENTS: (1) Octanedioic acid diethyl ester (diethyl octanedioate); $C_{12}H_{22}O_4$ ; [2050-23-9] (2) Water; $H_2O$ ; [7732-18-5] VARIABLES: T/K = 293 EXPERIMENTAL VALUES: The solubility of octanedioic acid di ported to be 0.068 g(1)/100mL(2). The	ORIGINAL MEASUREMENTS: Sobotka, H.; Kahn, J. J. Am. Chem. Soc. <u>1931</u> , 53, 2935-8. PREPARED BY: A. Skrzecz			
and 5.3 x $10^{-5}$ . Density of water $d_4^{20} = 0.9982$ (ref 1) was used in the calculation.				
AUXILIARY :	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra-	<ul> <li>(1) Source not specified (Eastman Kodak Laboratories or synthe- sized); twice-distilled under reduced pressure; d<sup>20</sup><sub>4</sub> 0.9822, n<sup>20</sup><sub>D</sub> 1.4334.</li> <li>(2) Distilled.</li> <li>ESTIMATED ERROR:</li> </ul>			
tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent droplets.	Not specified.			
	REFERENCES: 1. Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, 1973.			

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Decanoic acid ethyl ester	Sobotka, H.; Kahn, J.		
(ethyl decanoate); C <sub>12</sub> H <sub>24</sub> O <sub>2</sub> ;	J. Am. Chem. Soc. <u>1931</u> , 53,		
[110-38-3]	2935-8.		
(2) water; $H_20$ ; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 293	A. Skrzecz		
EXPERIMENTAL VALUES: The solubility of decanoic acid ethyl ester in water at 20°C was reported to be 0.0015 g(1)/100mL(2). The corresponding mass per cent and mole frac- tion, $x_1$ , values calculated by the compiler are 0.0015 g(1)/100g sln and 1.3 x 10 <sup>-6</sup> . Density of water $d_4^{20} = 0.9982$ (ref 1) was used in the calculation.			
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to convert the floating rough indica- tor particles into dark transparent droplets.	<ul> <li>(1) Source not specified (Eastman Kodak Laboratories or synthesized); twice-distilled under reduced pressure; d<sup>20</sup><sub>4</sub> 0.8637, n<sup>20</sup><sub>D</sub> 1.4269.</li> <li>(2) Distilled.</li> <li>ESTIMATED ERROR: Not specified.</li> </ul>		
arohiere.	REFERENCES: 1. Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, <u>1973</u> .		

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ol> <li>Dibutylphosphinic acid butyl ester         (butyl dibutylphosphinate);         C<sub>12</sub>H<sub>27</sub>O<sub>2</sub>P; [2950-47-2]         (2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ol>	<pre>Nikolaev, A.V.; Dyadin, Yu.A.; Yakolvlev, I.I.; Durasov, V.B.; Mironova, Z.N. Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk 1965, (3), 27-31.</pre>	
VARIABLES:	PREPARED BY:	
T/K = 273 - 429	A. Skrzecz	

EXPERIMENTAL VALUES:

Mutual solubility of dibutylphosphinic acid butyl ester and water

t/°C	g(1)/100g sln		x <sub>1</sub> (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0.		73.65 <sup>a</sup>		0.1769
3.7	1.30	-	$10.12 \times 10^{-4}$	-
6.1	-	75.46	-	0.1912
7.7	1.03	-	$8.00 \times 10^{-4}$	-
12.0	-	77.27	-	0.2072
14.4	0.716	-	5.54 x $10^{-4}$	-
17.5	-	78.54	-	0.2196
22.9	0.490	-	$3.78 \times 10^{-4}$	-
24.4	-	79.95	-	0.2346
25.0	0.49 <sup>b</sup>	80.45 <sup>a</sup>	$3.78 \times 10^{-4}$	0.2403
25.0	0.445	-	$3.44 \times 10^{-4}$	-
26.5	0.409	-	3.16 x $10^{-4}$	-
			(con	tinued next page)

AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The synthetic method proposed by Aleksejev was used. Light filters and a high intensity light source were used to measure the cloudiness point with good accuracy. As a check, two analytical methods were used: the Karl Fischer method for water in the organic phase and the extraction of dibutylphosphinic acid butyl ester with diethyl ether, stripping, and drying over  $P_2O_5$ . SOURCE AND PURITY OF MATERIALS:

- (1) Synthesized and purified as given by Nikolaev, Dyadin, Yakovlev and Mironova (ref 1); b.p.  $138^{\circ}C$  at 6 mm Hg,  $d_4^{20}$  0.9262,  $n_D^{20}$  1.4440.
- (2) Not specified.

ESTIMATED ERROR:

Temp.  $\pm (0.2-0.6)^{\circ}C$  below 30°C,  $\pm (1-3)^{\circ}C$  at high temperature.

**REFERENCES:** 

 Nikolaev, A.V.; Dyadin, Yu.A.; Yakovlev, I.I.; Mironova, Z.N. Dokl. Akad. Nauk SSSR <u>1963</u>, 153, 118.

COMPONENT	rs:		ORIGINAL MEASUREME	NTS:	
<ol> <li>Dibutylphosphinic acid butyl ester         (butyl dibutylphosphinate);         C<sub>12</sub>H<sub>27</sub>O<sub>2</sub>P; [2950-47-2]</li> <li>Water: H<sub>2</sub>O; [7732-18-5]</li> </ol>		<pre>Nikolaev, A.V.; Dyadin, Yu.A.; Yakolvlev, I.I.; Durasov, V.B.; Mironova, Z.N. Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk 1965, (3), 27-31.</pre>			
		-			
EXPERIMEN	NTAL VALUES: (co	ontinued) dibutylphosph	inic acid butyl est	er and water	
		arbucy rphosph	mic actu bucyl est	er and water	
$t/^{\circ}C$ g(1)/100g sln		0g sln	<pre>x1 (compiler)</pre>		
	(2)-rich phase	(1)-rich phase	e (2)-rich phase	(1)-rich phase	
31.5	0.341		$2.63 \times 10^{-4}$		
32.5	-	81.19	-	0.2492	
41.0	0.259	-	$2.00 \times 10^{-4}$	-	
43.2	-	82.38	-	0.2644	
55.0	-	83.29	-	0.2771	
57.5	0.200	-	$1.54 \times 10^{-4}$	-	
69.5	0.180	-	$1.39 \times 10^{-4}$	-	
70.7	_	84.12	-	0.2894	
87.0	0.180	-	$1.39 \times 10^{-4}$	-	
124.0	-	84.12	-	0.2894	
141.0	-	83.29	-	0.2771	
156.0	-	82.38	-	0.2644	

<sup>a</sup> Karl Fischer method.

<sup>b</sup> Extraction of dibutylphosphinic acid butyl ester with diethyl ether.

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<pre>COMPONENTS: (1) Dibutylphosphinic acid butyl     ester     (butyl dibutylphosphinate);     C<sub>12</sub>H<sub>27</sub>O<sub>2</sub>P; [2950-47-2] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Nikolaev, A.V.; Dyadin, Yu.A.; Yakovlev, I.I.; Durasov, V.B.; Yakovleva, N.I.; Khol'kina, I.D. Zh. Fiz. Khim. <u>1966</u> , 40, 221-3.
VARIABLES: T/K = 526	PREPARED BY: A. Skrzecz
The UCST was reported to be 253°C. The dibutylphosphinic acid butyl esten 150-170°C. The hydrolisis measured in ester after heating at 260°C through	er hydrolysis began at temperature a the sample containing 19.89wt% of 20 min was 5-10%.
AUXILIARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The Alekseev's synthetic method was used. A water or glycerine bath was used for temperature control. No further details were reported in the paper.	<ol> <li>(1) Synthesized; distilled 5-6 times under vacuum; d<sub>4</sub><sup>25</sup> 0.9179, n<sub>D</sub><sup>55</sup> 1.4442.</li> <li>(2) Not specified.</li> </ol>
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Butylphosphonic acid dibutyl ester (dibutyl butylphosphonate); C<sub>12</sub>H<sub>27</sub>O<sub>3</sub>P; [78-46-6]</li> <li>Water; H<sub>2</sub>O; [7732-18-5]</li> </ol>	<pre>Nikolaev, A.V.; Dyadin, Yu.A.; Yakolvlev, I.I.; Durasov, V.B.; Mironova, Z.N. Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk <u>1965</u>, (3), 27-31.</pre>
VARIABLES:	PREPARED BY:
T/K = 275 - 419	A. Skrzecz
EXPERIMENTAL VALUES:	

# Mutual solubility of butylphosphonic acid dibutyl ester and water

t/°C	g(1)/100g sln		$x_1$ (comp	iler)
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
2.2		86.00		0.3066
6.0	0.247	-	17.82 x 10 <sup>-5</sup>	-
13.3	-	87.47	-	0.3344
13.4	0.168	-	12.11 x 10 <sup>-5</sup>	-
20.5	-	88.12	-	0.3480
21.0	0.121	-	8.72 x 10 <sup>-5</sup>	-
24.1	-	88.44	-	0.3551
28.6	0.0985	-	7.10 x 10 <sup>-5</sup>	-
35.0	0.0853	-	6.14 x 10 <sup>-5</sup>	-
39.5	-	88.29	-	0.3750

(continued next page)

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The synthetic method proposed by (1) Synthesized and purified as given by Nikolaev, Dyadin, Yakovlev and Mironova (ref 1); Aleksejev was used. Light filters and a high intensity light source were used to measure the cloudiness b.p.  $133-5^{\circ}C$  at 6 mm Hg,  $d_4^{20}$  0.9472,  $n_D^{20}$  1.4323. point with good accuracy. No further details were reported in the paper. (2) Not specified. ESTIMATED ERROR: Temp.  $\pm (0.2-0.6)^{\circ}C$  below  $30^{\circ}C$ ,  $\pm(1-3)^{\circ}C$  at high temperature. **REFERENCES:**  Nikolaev, A.V.; Dyadin, Yu.A.; Yakovlev, I.I.; Mironova, Z.N. Dokl. AKad. Nauk SSSR <u>1963</u>, 153, 118.

<pre>COMPONENTS: (1) Butylphosphonic acid dibutyl     ester     (dibutyl butylphosphonate);     C<sub>12</sub>H<sub>27</sub>O<sub>3</sub>P; [78-46-6] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>		ORIGINAL MEASUREME Nikolaev, A.V.; D Yakolvlev, I.I. Mironova, Z.N. Izv. Sib. Otd. Ak Ser. Khim. Nauk 27-31.	NTS: yadin, Yu.A.; ; Durasov, V.B.; ad. Nauk SSSR, <u>1965</u> , (3),	
EXPERIMEN Mutua 	TAL VALUES: (co l solubility of  g(1)/10 (2)-rich phase	ontinued) butylphosphor 	nic acid dibutyl est 	er and water iler) (1)-rich phase
43.9	0.0688	-	4.95 x 10 <sup>-5</sup>	_
48.0	0.0591	-	4.26 x 10 <sup>-5</sup>	-
51.8	-	89.76	-	0.3868
96.0	-	89.76	-	0.3868
100.0	0.0591	-	4.26 x 10 <sup>-5</sup>	-
106.0	0.0688	-	$4.95 \times 10^{-5}$	-
109.0	-	88.29	-	0.3750
126.0	-	88.44	-	0.3551
146.0	-	87.47	-	0.3344

сомро	NENTS:	EVALUATOR:
(1)	Phosphoric acid tributyl ester	G.T. Hefter, School of Mathematical
(tributyl phosphate);		and Physical Sciences,
	C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P; [126-73-8]	Murdoch University, Perth, W.A.,
(2) Water: $H_{-0}$ : [7732-18-5]	Australia	
(2)		December, 1988

CRITICAL EVALUATION:

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

<u>TABLE 1: Quar</u> Phosphoric acid	titative_Sol tributyl_este	<u>ubility Studies</u> er (1) - Water (1	<u>of the</u> 2) System
Reference	T/K	Solubility	Method
Alcock et al. (ref 1)	289-298	mutual	analytical
Burger and Forsman (ref 2)	293	mutual	unspecified
Higgins et al. (ref 3)	277-323	(1) in (2)	analytical
Hasegawa (ref 4)	298	(1) in (2)	titration
Mikhailov <i>et al</i> . (ref 5)	279-299	(2) in (1)	Karl Fischer, synthetic
Hardy et al. (ref 6)	273-333	(2) in (1)	Karl Fischer
Nikolaev et al. (ref 7)	273-460	mutual	Karl Fischer, synthetic

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. SOLUBILITY OF PHOSPHORIC ACID TRIBUTYL ESTER (1) IN WATER (2)

All the available data for the solubility of phosphoric acid tributyl ester (1) in water (2) are summarized in Table 2 with the following exceptions. The data of Alcock et al. (ref 1) are much lower, and that of Hasegawa (ref 4) much higher, than all other studies and have therefore been rejected.

Agreement among the remaining data (Table 2) is in general good and a number of the average "Best" values have been Recommended. At higher temperatures (T > 323 K) only the data of Nikolaev (ref 7) are available and must therefore be considered as Tentative. Selected data are plotted in Figure 1.

(continued next page)

COMPC	DNENTS:	EVALUATOR:
<ol> <li>Phosphoric acid tributyl ester (tributyl phosphate); C<sub>12</sub>H<sub>27</sub>O<sub>4</sub>P; [126-73-8]</li> <li>Water; H<sub>2</sub>O; [7732-18-5]</li> </ol>		G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988
CRITI	ICAL EVALUATION: (continued)	
		·
	TABLE 2: Recommended (R)	and Tentative Solubilities
	or Phosphoric acia tribut	yi ester (1) in water (2)
T/K	Sol	lubilities
	Reported values	"Best" values $(\pm \sigma_n)^a$
	10 <sup>2</sup> g(1)/100g sln	$10^2$ g(1)/100g sln $10^5 x_1$
283	7.5 <sup>*</sup> (ref 3), 7.5 <sup>*</sup> (ref 7	) 7.5 (R) 5.1
293	4.8 <sup>*</sup> (ref 3), 4.6 <sup>*</sup> (ref 7	) 4.7 ± 0.1 (R) 3.2
298	3.9 (ref 2), $4.2^*$ (ref 3)	, 4.0 ± 0.1 (R) 2.7
303	3.8 <sup>*</sup> (ref 3), 3.5 <sup>*</sup> (ref 7	) $3.7 \pm 0.2$ (R) $2.5$
313	3.4 <sup>*</sup> (ref 3), 2.9 <sup>*</sup> (ref 7	) 3.2 ± 0.3 2.2
323	2.9 <sup>*</sup> (ref 3), 2.6 <sup>*</sup> (ref 7	) 2.8 ± 0.2 1.9
333	2.5 <sup>*</sup> (ref 7)	2.5 1.7
343	2.6 <sup>*</sup> (ref 7)	2.6 1.8
353	2.9 <sup>*</sup> (ref 7)	2.9 2.0

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_1)$  have the same status and (relative) percentage uncertainties as the mass % solubilities.

3.6

5.0

2. SOLUBILITY OF WATER (2) IN PHOSPHORIC ACID TRIBUTYL ESTER (1)

363

373

3.6<sup>\*</sup> (ref 7)

5.0<sup>\*</sup> (ref 7)

All the available data for the solubility of water (2) in phosphoric acid tributyl ester (1) are summarized in Table 3 with the exception of the datum of Alcock *et al.* (ref 1) which is lower than all other studies and has therefore been rejected.

The remaining data are in good agreement (Table 3) enabling a number of average "Best" values to be Recommended. At higher temperatures (T >343 K) only the data of Nikolaev (ref 7) are available and must therefore be considered as Tentative. Selected data are plotted in Figure 2.

2.5

3.4





COMPONENTS:	EVALUATOR:
<ol> <li>Phosphoric acid tributyl ester (<i>tributyl phosphate</i>); C<sub>12</sub>H<sub>27</sub>O<sub>4</sub>P; [126-73-8]</li> <li>Water; H<sub>2</sub>O; [7732-18-5]</li> </ol>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988

CRITICAL EVALUATION: (continued)

## TABLE 3: Recommended (R) and Tentative Solubilities of Water (2) in Phosphoric acid tributyl ester (1)

T/K	Solubilit	ies	
	Reported values	"Best" values $(\pm \sigma_n)$	a
	g(2)/100g sln	g(2)/100g sln	<i>x</i> <sub>2</sub>
273	7.09 (ref 6), 7.52 (ref 7)	7.3 ± 0.2 (R)	0.54
283	6.38 <sup>*</sup> (ref 5), 6.92 <sup>*</sup> (ref 6), 7.05 <sup>*</sup> (ref 7)	6.8 ± 0.3 (R) 0	0.52
293	6.24 <sup>*</sup> (ref 5), 6.73 <sup>*</sup> (ref 6), 6.70 <sup>*</sup> (ref 7)	6.6 ± 0.2 (R) 0	0.51
298	6.24 (ref 5), 6.64 (ref 6), 6.56 (ref 7)	6.5 ± 0.2 (R) 0	0.51
303	6.53 <sup>*</sup> (ref 6), 6.45 <sup>*</sup> (ref 7)	6.49 ± 0.04 (R)	0.507
313	6.31 <sup>*</sup> (ref 6), 6.40 <sup>*</sup> (ref 7)	6.36 ± 0.05 (R)	0.501
323	6.08 (ref 6), 6.37 <sup>*</sup> (ref 7)	6.2 ± 0.1 (R)	0.49
333	5.82 (ref 6), 6.40 <sup>*</sup> (ref 7)	6.1 ± 0.3 (R) 0	0.49
343	6.60 <sup>*</sup> (ref 7)	6.6 0	0.51
353	6.85 <sup>*</sup> (ref 7)	6.9 (	0.52
363	7.17 <sup>*</sup> (ref 7)	7.2 0	0.53
373	7.55 <sup>*</sup> (ref 7)	7.6	0.55
393	8.40 <sup>*</sup> (ref 7)	8.4 0	0.58
413	9.3 <sup>*</sup> (ref 7)	9 (	0.59
433	10.1 <sup>*</sup> (ref 7)	10 0	0.62
453	10.9 <sup>*</sup> (ref 7)	11 (	0.65

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities ( $x_2$ ) have the same status and (relative) percentage uncertainties as the mass % solubilities.

(continued next page)



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COMPONENTS:		ORIGINAL MEASUREMENTS:
<ol> <li>Phosphoric acid tributyl ester (tributyl phosphate);</li> </ol>		Alcock, K.; Grimley, S.S.; Healy, T.V.; Kennedy, J.; McKay, H.A.C.
C <sub>12</sub> H <sub>27</sub>	,0 <sub>4</sub> P; [126-73-8]	Trans. Faraday Soc. <u>1956</u> , 52,
(2) Water	; H <sub>2</sub> O; [7732-18-5]	39-47.
VARIABLES:		PREPARED BY:
T/K = 289	- 298	A. Skrzecz
EXPERIMENTA	L VALUES:	
Solubilit	y of phosphoric acid tribut	tyl ester in water
t/°C	g(1)/dm <sup>3</sup> mc	pl(1)/dm <sup>3</sup> sln
		(compiler)
16.	0.420	0.001577
17.	0.410	0.001540
19.	0.397	0.001491
22.	0.380	0.001427
Solubility  t/°C	y of water in phosphoric ad mol(1)/dm <sup>3</sup> sln	cid tributyl ester  g(2)/dm <sup>3</sup> sln (compiler)
25.	3.22	58.0
25.	3.43	61.8
	AUXILIARY	INFORMATION
METHOD/APPAP	RATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. 0.5 cm <sup>3</sup> of <sup>32</sup> P-labelled organic phase was shaken with 50 cm <sup>3</sup> of aq. phase for 20 min. After a short standing period, the aqueous phase was separated and centrifuged. A sample was diluted 10-fold, and 10 cm <sup>3</sup> were placed in a GM6 liquid counter for counting and comparison with a suitable standard. The method was reported together with the systems phosphoric acid tri- butyl ester-water-diluent-nitric acid.		<ul> <li>(1) Source not specified; purified by boiling with dilute NaOH solution to distill volatile impurities; the remaining portion washed repeatedly with water. <sup>32</sup>P-labelled (1) supplied by Radiochemical Center, Amersham; purified as described above.</li> <li>(2) Not specified.</li> <li>ESTIMATED ERROR: Not specified.</li> </ul>
		REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Phosphoric acid tributyl ester (tributyl phosphate); C<sub>12</sub>H<sub>27</sub>O<sub>4</sub>P; [126-73-8]</pre>	Burger, L.L.; Forsman, R.C. Report HW-20936, 1951. Data taken from: Bruce, F.R.; Flotchor, J.M., Human, W.W.	
(2) Water; H <sub>2</sub> O; [7732-18-5]	Fletcher, J.M.; Hyman, H.H. Progress in Nuclear Energy, ser.3, Process Chemistry vol.2, Pergamon Press, <u>1958</u> , 546-56.	
VARIABLES:	PREPARED BY:	
T/K = 298	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of phosphoric acid tributyl ester in water at 25°C was re- ported to be 0.39 g(1)/dm <sup>3</sup> sln. The corresponding value on a mole/volume basis is 0.00146 mol(1)/dm <sup>3</sup> . The solubility of water in phosphoric acid tributyl ester at 25°C was re- ported to be 64 g(2)/dm <sup>3</sup> sln. The corresponding value on a mole/volume basis is 3.55 mol(2)/dm <sup>3</sup> sln.		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Not specified.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	ESTIMATED ERROR: Not specified.	
	ESTIMATED ERROR: Not specified.	

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COMPONENTS:		ORIGINAL MEASUREMENTS:
<pre>(1) Phosphoric acid tributyl ester (tributyl phosphate);</pre>		Higgins, C.E.; Baldwin, W.H.; Soldano, B.A.
C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P; [126-73-8]		J. Phys. Chem. <u>1959</u> , 63, 113-8.
(2) Water	; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:		PREPARED BY:
T/K = 277	- 323	A. Skrzecz
FYDEDIMENTA	I. VALUES.	I
Solubilit	y of phosphoric acid tribut	cyl ester in water
t/°c	mg(1)/dm <sup>3</sup> sln mo	l(1)/dm <sup>3</sup> sln
3.4	1075	0.0040
4.0	1012	0.0038 <sup>b</sup>
5.0	957	0.0036 <sup>b</sup>
13.0	640	0.0024 <sup>b</sup>
25.0	422 <sup>a</sup>	0.0016
50.0	285	0.0011
<u></u> ,	AUXILIARY	INFORMATION
METHOD/APPAI	RATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The mixture of water and ester labeled with <sup>32</sup> P were tumbled in a constant temperature bath for 1/2 to 1 h. and stored overnight to ensure com- plete separation. The aqueous phase was analysed by counting a dilution of an aliquot containing sufficient activity in the solution counter as described by Higgins and Baldwin (ref 1). The specific activity of the labeled ester was measured at the same time for comparison. The averages of at least two separated determinations were presented.		<ul> <li>(1) Source not specified, C.P. grade; tributyl phosphate-<sup>32</sup>P prepared in the laboratory as described by Higgins and Baldwin (ref 2); specific activity 40-50(micro)c/mmole.</li> <li>(2) Not specified.</li> <li>ESTIMATED ERROR: Temp. ±0.2°C. Soly. ±1.8% (the largest average deviation of a single determination at 25°C).</li> </ul>
		<pre>REFERENCES: 1. Higgins, C.E.; Baldwin, W.H. Anal. Chem. <u>1955</u>, 27, 1780. 2. Higgins, C.E.; Baldwin, W.H. J. Org. Chem. <u>1956</u>, 21, 1156.</pre>
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phosphoric acid tributyl ester	Hasegawa T.
(tributyl phosphate); C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P; [126-73-8]	Kogyo Kagaku Zasshi <u>1961</u> , 64(7), 1239-41.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of phosphoric acid tributyl ester in water $25^{\circ}C$ was reported to be 6.8 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calculated by the compiler is 0.0049.	
AUXILIARY INFORMATION	
METHOD / APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. The cloudiness was observed visually. The data and method were reported together with the ternary systems phosphoric acid tributyl ester- water-2-furancarbonal (tributyl phosphate-water-furfural). No fur- ther details were reported in the paper.	<pre>(1) Source not specified; boiled with 5 volumes of 0.4% NaOH(aq) washed several times with water, distilled at reduced pressure; b.p. 132°C at 9 mm Hg, d<sub>4</sub><sup>25</sup> 0.9538. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:</pre>
	203
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COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Phosphoric acid tributyl ester (tributyl phosphate);</li> </ol>	Mikhailov, V.A.; Kharchenko, S.K.; Nazin, A.G.
C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P; [126-73-8] (2) Water; H <sub>2</sub> O; [7732-18-5]	Izv. Sib. Otd. Akad. Nauk SSSR <u>1962</u> , (7), 50-6.
VARTARLES.	PREDARED BY.
T/K = 279 - 299	A. Skrzecz
EXPERIMENTAL VALUES: Solubility of water in phosphoric a	acid tributyl ester
t/°C g(2)/100g sln	x <sub>2</sub> (compiler)
5.5 <sup>b</sup> 6.37	0.501
17. <sup>b</sup> 6.25	0.496
25. <sup>a</sup> 6.244(0.014) <sup>d</sup>	0.4961(0.0005) (authors)
25.° 6.38	0.502
26. <sup>b</sup> 6.22	0.495
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical, Alekseev's synthe- tic, and the isopieztic methods were used. In the analytical method, the phases were separated, after thermostating 2-3 h., using a	<ul> <li>(1) Source not specified; distilled at vacuum over solid Na<sub>2</sub>CO<sub>3</sub>; d<sub>4</sub><sup>25</sup> 0.9728, n<sub>D</sub><sup>25</sup> 1.4244.</li> <li>(2) Not specified.</li> </ul>
accurate results), and the water	
reagent. For the Alekseev's method,	ESTIMATED ERPOR.
sealed ampoules containing a known sample composition along with a	
magnetic stirrer were placed into a water bath and the temperature of cloudiness was observed. In the isopiestic procedure, the assump-	Temp. $\pm 0.05^{\circ}C^{\circ}$ and $\pm (1-2)^{\circ}C^{\circ}$ .
tion that the ester phase was in equilibrium with pure water was made. No further details were pro- vided in the paper.	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Phosphoric acid tributyl ester (tributyl phosphate); CoeHerQ.P: [126-73-8]	Hardy, C.J.; Fairhurst, D.; McKay, H.A.C.; Willson, A.M.		
(2) Water: $H_0$ ; [7732-18-5]	1626-36.		
VARIABLES:	PREPARED BY:		
T/K = 273 - 333	A. Skrzecz		
EXPERIMENTAL VALUES: Solubility of water in phosp	noric acid tributyl ester		
t/°C mol(2)/dm <sup>3</sup> sln density g/cm <sup>3</sup>	$g(2)/100g sln x_2$ (compiler) (compiler)		
$0.(0.2)$ $3.92$ $0.9982$ $25.(0.2)$ $3.59(0.03)^a$ $0.9760$ $40.(0.1)$ $3.34$ $0.9640$ $50.(0.1)$ $3.23$ $0.9573^b$ $60.(0.1)$ $3.07$ $0.9508^b$	7.09       0.5296         6.64       0.5120         6.26       0.4960         6.08       0.4889         5.82       0.4773		
with water vapour. <sup>b</sup> Calculated from authors' equation: $d_t = 0.9982 (1.0 - 9.6 \times 10^{-4} (t/^{\circ}C) + 2.8 \times 10^{-6} (t/^{\circ}C)^2)$			
AUXILIARY	INFORMATION		
<pre>METHOD/APPARATUS/PROCEDURE: The analytical method was used. The solutions were prepared by shaking together known weights of compo- nents for 15 min or by saturating ester with steam. The ester was equilibrated with water at 25°C by: (i) shaking in a mechanical shak- er for 15 minutes and centri- fuged, (ii) stirring 10 cm<sup>3</sup> of each phase in 2 40 cm<sup>3</sup> contrifuce tube</pre>	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer- cially available; washed and heated with 0.1 N alkali, volatile matter distilled in a stream of nitrogen, the remaining alkaline solution washed six times with water, dried under vacuum at 40-50°C with a nitrogen bleed, stored in a dark glass stoppered</pre>		

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COMPONENT	s:		ORIGINAL MEASUREMEN	ITS:
<pre>(1) Phosphoric acid tributyl ester (tributyl phosphate); C<sub>12</sub>H<sub>27</sub>O<sub>4</sub>P; [126-73-8]</pre>		Nikolaev, A.V.; Dy Yakolvlev, I.I.; Mironova, Z.N. Izv. Sib. Otd. Aka	<pre>vadin, Yu.A.; Durasov, V.B.; vd. Nauk SSSR, 1965 (2)</pre>	
(2) Wat	er; H <sub>2</sub> O; [//32-	18-2]	27-31.	<u>1965</u> , (3),
VARIABLES:		PREPARED BY:	۰	
T/K = 273 - 460		A. Skrzecz		
EXPERIMEN <sup>®</sup> Mutua	TAL VALUES: al solubility o	f phosphoric a	acid tributyl ester a	and water
t/°C	g(1)/1 (2)-rich phase	00g sln (1)-rich phas	x <sub>1</sub> (compi se (2)-rich phase (	ler) (1)-rich phase
0. <sup>a</sup>		92.48		0.4541
4.6	-	92.70	-	0.4621
5.4	0.0994	-	6.73 x 10 <sup>-5</sup>	-
9.1	-	92.89	-	0.4692
13.9	0.0620	-	$4.20 \times 10^{-5}$	_
14.6	_	93.09	-	0.4756
16 3	_	93.18	_	0.4903
10.2	0 0474	-	2 21 2 10-5	0.4005
19.3	0.0474	-	3.21 X 10	-
21.6	-	93.33	-	0.4863
24.2	-	93.38	-	0.4883
24.7	0.0403	-	2.73 X 10 5	-
25.04	-	93.44	- (cont	inued next page)
		ΔΙΙΥΤΙ.ΤΑΡΥ	ТИЕОРМАТТОИ	
			COURCE AND DUDING	
ETHOD/API	PARATUS/PROCEDU	KE:	SOURCE AND PURITY O	F MATERIALS:
The synthetic method proposed by Aleksejev was used. Light filters and a high intensity light source were used to measure the cloudiness point with good accuracy. The Karl Fischer analytical method was used as a check. No further details were reported in the paper.		(1) Source not spe grade; washed with NaOH(aq), $H_2O$ , three tim under vacuum; at 3 mm Hg, $d_4^2$ $n_D^{25}$ 1.4224.	cified, pure several times diluted HCL, es distilled b.p. 132-3°C <sup>5</sup> 0.9723,	
		(2) Not specified.		
			ESTIMATED ERROR:	
		i	Temp. ±(0.2-0.6)°C ±(1-3)°C at 1	below 30 <sup>0</sup> C, high temperature.
			REFERENCES:	

COMPONENTS:		ORIGINAL MEASUREMEN	NTS:	
<ol> <li>Phosphoric acid tributyl ester (<i>tributyl phosphate</i>); C<sub>12</sub>H<sub>27</sub>O<sub>4</sub>P; [126-73-8]</li> <li>Water; H<sub>2</sub>O; [7732-18-5]</li> </ol>		Nikolaev, A.V.; Dy Yakolvlev, I.I.; Mironova, Z.N. Izv. Sib. Otd. Aka Ser. Khim. Nauk 27-31.	yadin, Yu.A.; Durasov, V.B.; ad. Nauk SSSR, <u>1965</u> , (3),	
EXPERIMEN	TAL VALUES: (c	ontinued)		
Mut	ual solubility	of phosphoric	acid tributyl ester	and water
. <u> </u>				
t/°C	g(1)/1	00g sln	$x_1$ (compi	ller)
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase
25.1	-	93.41	-	0.4895
25.3	-	93.46	-	0.4915
29.5	-	93.52	-	0.4940
33.1	0.0329	-	$2.23 \times 10^{-5}$	-
34.2	-	93.58	-	0.4965
39.2	0.0292	-	1.98 x 10 <sup>-5</sup>	-
60.2	-	93.58	-	0.4965
65.0	-	93.52	-	0.4940
69.5	-	93.41	-	0.4895
71.0	-	93.38	-	0.4883
78.0	-	93.18	-	0.4803
80.8	0.0292	-	1.98 x 10 <sup>-5</sup>	-
82.0	-	93.09	-	0.4756
86.0	0.0329	-	2.23 x 10 <sup>-5</sup>	-
94.5	0.0403	92.70	$2.73 \times 10^{-5}$	0.4621
106.0	-	92.22	-	0.4450
117.0	-	91.72	-	0.4284
131.0	-	92.77	-	0.4646
134.0	-	89.02	-	0.3542
187.0	-	88.77	-	0.3484

a Karl Fischer analytical method.

	1
COMPONENTS:	ORIGINAL MEASUREMENTS:
propyl) ester (tri(2-methyl-	Apelblat, A.
propyl) phosphate); $C_{12}H_{27}O_AP$ ;	J. Chem. Soc. B <u>1969</u> , 175-7.
[126-71-6]	
(2) Water: H_O: [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of water in phosphorid 25°C was reported to be 3.50 mol(2)/I mole/volume basis is 63.1 g(2)/L sln The density of the ester-phase was re	c acid tris(2-methylpropyl) ester at 5 sln. The corresponding value on a (compiler). eported was to be $d^{25}$ 0.9655.
AUXILJARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The mixture was equilibrated by vigor- ous stirring for 30 min. and settl- ing for 12 h. The organic phase was analyzed with the Karl Fischer rea- gent. Preliminary experiments show- ed that stirring and settling times were sufficient.	<ul> <li>(1) Albright and Wilson Co; purified by method described in (ref 1); d<sub>4</sub><sup>25</sup> 0.9614, n<sub>D</sub><sup>25</sup> 1.4168.</li> <li>(2) Not specified.</li> <li>ESTIMATED ERROR: Temp. ±0.1°C.</li> <li>REFERENCES:</li> <li>1. Alcock, K.; Grimley, S.S.; Healy, T.V.; Kennedy, J.; McKay.</li> </ul>
	H.A.C. Trans. Faraday Soc. <u>1956</u> , 52, 39.

COMPONENTS:	EVALUATOR:
<ul> <li>(1) Benzoic acid, 2-hydroxy-, phenyl ester         (phenyl salicylate); C<sub>13</sub>H<sub>10</sub>O<sub>3</sub>;         [118-55-8]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia March, 1990

CRITICAL EVALUATION:

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

<u>TABLE 1: Quantitative Solubility Studies of the</u> 2-Hydroxybenzoic acid phenyl ester (1) - Water (2) System			
Reference	т/к	Solubility	Method
		g(1)/100 g sln	
Seidell (ref 1)	298	0.015	gravimetric
Dehn (ref 2)	$RT^{a}$	0.04	gravimetric

a Room temperature (293-298 K).

As can be seen from Table 1, the data of Seidell (ref 1) and Dehn (ref 2) for the solubility of phenyl salicylate (1) in water (2) are not in particularly good agreement. In the absence of further information it is not possible to prefer either value although it may be noted that Seidell's data in other systems are generally close to Recommended values.

### REFERENCES

- Seidell, A. Hygienic Lab. Bull. <u>1910</u>, No. 67, 98pp. (U.S. Govt. Printing Office, Washington, DC).
- 2. Dehn, W. M. J. Am. Chem. Soc. <u>1917</u>, 39, 1399-404.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzoic acid, 2-hydroxy-,	Seidell, A.
phenyl ester	Hygienic Lab. Bull. <u>1910</u> , No. 67,
(pnenyi salicylate);	98 nn (US Covt Printing Office
(2) Water; H <sub>2</sub> O; [7732-18-5]	Washington, DC).
VARIABLES:	PREPARED BY:
T/K = 298	G.T. Hefter
The solubility of 2-hydroxybenzoic ac reported to be 0.015 g(1)/100g sln. 7 value calculated by the compiler is 1	cid phenyl ester in water at 25°C was The corresponding mole fraction, x <sub>1</sub> , 1.3 x 10 <sup>-5</sup> .
-	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. Appropriate quantities of (1) and (2) were shaken together for two days. The amount of dissolved (1) was determined by evaporation of a known quantity of the saturated solution. The residue was dried to a constant weight in a vacuum desiccator.	<ul> <li>(1) Source not stated; purity determined to be practically 100% by saponification.</li> <li>(2) Distilled (no details given).</li> <li>ESTIMATED ERROR:</li> <li>Temp. not stated.</li> <li>Soly. not stated.</li> </ul>

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzoic acid, 2-hydroxy-,	Dehn, W.M.
(nhonyl saligulate): C. H. O.	J. Am. Chem. Soc. <u>1917</u> , 39,
$(p_{118-55-8})$	1399-1404.
(2) Water; $H_20$ ; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = room temperature	A. Skrzecz
EXPERIMENTAL VALUES:	
The solubility of 2-hydroxybenzoic ac	bid phenyl ester in water at room tem-
perature <sup>a</sup> was reported to be 0.04 g(1	)/100g(1). The corresponding mass
percentage and mole fraction, $x_1$ , val	ues calculated by the compiler are
0.040 g(1)/100g sln and 3.4 x $10^{-5}$ .	
a Deem termenture use reserved to	ba 20.2590
- Room temperature was reported to	be 20-25-C.
AUXILIARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Excess of the substance and 5 mL of	(1) Source not specified, commer-
which, when stoppered, were shaken	cial grade; used as received.
or were left until equilibrium was established. The solutions were	(2) Not specified.
filtered into weighed crucibles and	
desiccator or on a water bath, the	
crucibles were again weighed and the loss of solvent calculated. The	ESTIMATED ERROR:
measurements were made at room tem-	Not specified.
peracures from 20 to 25 t.	• • • • • • • • • • • • • • • • • • • •
	REFERENCES:

COMPONENTS: (1) Phosphoric acid methyl diphenyl ester	ORIGINAL MEASUREMENTS: Apelblat, A.
(methyl diphenyl phosphate); C <sub>13</sub> H <sub>13</sub> O <sub>4</sub> P; [115-89-9]	J. Chem. Soc. B <u>1969</u> , 175-7.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of water in phosphoric was reported to be 1.49 mol(2)/L sln mass/volume basis is 26.8 g(2)/L sln The density of the ester-phase was re	c acid methyl diphenyl ester at 25°C . The corresponding value on a (compiler). eported was to be d <sup>25</sup> 1.2195.
AUXTLTARY	
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The mixture was equilibrated by vigor- ous stirring for 30 min. and settl- ing for 12 h. The organic phase was analyzed with the Karl Fischer rea- gent. Preliminary experiments show- ed that stirring and settling times	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Aldrich Chemical Co.; purified by method described by Alcock, Grimley, Healy, Kennedy and McKay (ref 1); d<sub>4</sub><sup>25</sup> 1.2258, n<sub>D</sub><sup>25</sup> 1.5356.</li> <li>(2) Not specified.</li> </ul>
	ESTIMATED ERROR:
	Temp. ±0.1 <sup>0</sup> C.
	REFERENCES: 1. Alcock, K.; Grimley, S.S.; Healy, T.V.; Kennedy, J.; McKay, H.A.C. Trans. Faraday Soc. <u>1956</u> , 52, 39.

	<b>1</b>	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Nonanedioic acid diethyl ester (diethyl nonanedioate);</pre>	Sobotka, H.; Kahn, J.	
	J. Am. Chem. Soc. <u>1931</u> , 53,	
$C_{13}H_{24}O_4$ ; [624-17-9]	2935-8.	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of nonanedioic acid diported to be 0.025 g(1)/100mL(2). The fraction, $x_1$ , values calculated by thand 1.8 x 10 <sup>-5</sup> . Density of water $d_4^{20} = 0.9982$ (ref 1)	iethyl ester in water at 20°C was re- e corresponding mass per cent and mole ne compiler are 0.025 g(1)/100g sln was used in the calculation.	
AUXTLTARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. The ester was added dropwise from a micro-burette with a capillary tip to 100, 250, or 500 mL of water in a narrow-mouthed stock bottle with a well-ground glass stopper. The bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV dye was put into the water to im- prove the end-point of the titra- tion. At saturation, one additional drop of ester was sufficient to	<ul> <li>(1) Source not specified (Eastman Kodak Laboratories or synthesized); twice-distilled under reduced pressure; d<sup>20</sup><sub>4</sub> 0.9729, n<sup>20</sup><sub>D</sub> 1.4358.</li> <li>(2) Distilled.</li> <li>ESTIMATED ERROR: Not specified.</li> </ul>	
convert the floating rough indica- tor particles into dark transparent		
droplets.	REFERENCES:	
	<ol> <li>Selected Values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, <u>1973</u>.</li> </ol>	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 1,2-Benzenedicarboxylic acid	Leyder, F.; Boulanger, P.	
di-2-propenyl ester	Bull. Environ. Contam. Toxicol.	
(131-17-9)	<u>1983</u> , 30(2), 152-7.	
$(2)  \text{Waters} = H_{0} \cdot [7722 - 18 - 5]$		
$(2)$ water; $n_20$ ; $[7/32-18-5]$		
	DEEDIDED BY.	
T/K = 293	A. SKrzecz	
EXPERIMENTAL VALUES: The solubility of 1,2-benzenedicarbox water at 20°C was reported to be 7.39	<pre>xylic acid di-2-propenyl ester in &gt; x 10<sup>-4</sup> mol(1)/L and 0.182 g(1)/L.</pre>	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The analytical method as described in the OECD Guidelines for Testing of Chemicals (ref 1) was used. Gas chromatography analyses were con- ducted on a Girdel 3000 FFLE ap- paratus with flame-ionization de- tection. A 4 mm x 180 m stainless	<ol> <li>(1) CEPEA; purity not specified; used as received.</li> <li>(2) Deionized and distilled from KMnO<sub>4</sub>.</li> </ol>	
80-100 mesh Chromosorb W-AW-DMCS	ESTIMATED ERROR:	
were used. Samples were fortified	Temp. ±1°C.	
with an internal standard, extract- ed, and concentrated to 1 mL of hexane solution. "Solvent flush" and "hot needle" injection tech-		
gave similar results. Peak heights	REFERENCES:	
urements were made by using 1-cm cells in a Perkin-Elmer model 552 uv-Visible spectrophotometer.	1. OECD Guidelines for Testing of Chemicals, Paris, OECD, <u>1981</u> . (methods 101, 105).	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ul> <li>(1) 1,2-Benzenedicarboxylic acid bis(1-methylethyl) ester (diisopropyl phthalate); C<sub>14</sub>H<sub>18</sub>O<sub>4</sub>; [605-45-8]</li> <li>(2) Water: H<sub>2</sub>O; [7732-18-5]</li> </ul>	Leyder, F.; Boulanger, P. Bull. Environ. Contam. Toxicol. <u>1983</u> , 30(2), 152-7.
$(2)$ water, $n_20$ , $[7732-10-5]$	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
The solubility of 1,2-benzenedicarbox water at 20 <sup>o</sup> C was reported to be 1.33	xylic acid bis(1-methylethyl) ester in 3 x 10 <sup>-3</sup> mol(1)/L and 0.332 g(1)/L.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The analytical method as described in the OECD Guidelines for Testing of Chemicals (ref 1) was used. Gas chromatography analyses were con- ducted on a Girdel 3000 FFLE ap- paratus with flame-ionization de- tection. A 4 mm x 180 m stainless steel column packed with 3% OV-1 on 80-100 mesh Chromosorb W-AW-DMCS and helium at a 20mL/min flow rate were used. Samples were fortified with an internal standard, extract- ed, and concentrated to 1 mL of hexane solution. "Solvent flush" and "hot needle" injection tech- niques were used. The two methods gave similar results. Peak heights were measured throughout. UV meas- urements were made by using 1-cm cells in a Perkin-Elmer model 552 uv-Visible spectrophotometer.	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Chrompack, stationary phase for gas chromatography; used as received.</li> <li>(2) Deionized and distilled from KMnO<sub>4</sub>.</li> <li>ESTIMATED ERROR: Temp. ±1°C.</li> </ul>
	REFERENCES: 1. OECD Guidelines for Testing of Chemicals, Paris, OECD, <u>1981</u> . (methods 101, 105).

<pre>COMPONENTS: (1) 1,2-Benzenedicarboxylic acid     dipropyl ester     (dipropyl phthalate); C<sub>14</sub>H<sub>18</sub>O<sub>4</sub>;     [131-16-8] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Leyder, F.; Boulanger, P. Bull. Environ. Contam. Toxicol. <u>1983</u> , 30(2), 152-7.
VARIABLES: T/K = 293	PREPARED BY: A. Skrzecz
EXPERIMENTAL VALUES:	

The solubility of 1,2-benzenedicarboxylic acid dipropyl ester in water at  $20^{\circ}$ C was reported to be 4.32 x  $10^{-4}$  mol(1)/L and 0.108 g(1)/L.

AUXILIARY	INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The analytical method as described in the OECD Guidelines for Testing of Chemicals (ref 1) was used. Gas chromatography analyses were conducted on a Girdel 3000 FFLE apparatus with flame-ionization detection. A 4 mm x 180 m stainless steel column packed with 3% OV-1 on 80-100 mesh Chromosorb W-AW-DMCS and helium at a 20mL/min flow rate were used. Samples were fortified with an internal standard, extracted, and concentrated to 1 mL of hexane solution. "Solvent flush" and "hot needle" injection techniques were used. The two methods gave similar results. Peak heights were measured throughout. UV measurements were made by using 1-cm cells in a Perkin-Elmer model 552 uv-Visible spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

- Chrompack, stationary phase for gas chromatography; used as received.
- (2) Deionized and distilled from KMnO<sub>4</sub>.

ESTIMATED ERROR:

Temp. ±1°C.

#### **REFERENCES:**

1. OECD Guidelines for Testing of Chemicals, Paris, OECD, <u>1981</u>. (methods 101, 105).

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Decanedioic acid diethyl ester	Sobotka, H.; Kahn, J.	
(diethyl decanedioate);	J. Am. Chem. Soc. <u>1931</u> , 53, 2935-8	
(2) Water: $H_{0}$ ; [7732-18-5]	2555 0.	
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES:		
The solubility of decanedicic acid dietnyl ester in water at 20°C was reported to be $0.008 \text{ g}(1)/100\text{mL}(2)$ . The corresponding mass per cent and mole		
fraction, $x_1$ , values calculated by the compiler are 0.008 g(1)/100g sln		
and 6 x $10^{-6}$ .		
Density of water $d_{4}^{20} = 0.9982$ (ref 1) was used in the calculation.		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. The ester was added dropwise from a	(1) Source not specified (Eastman Kodak Laboratories or synthe-	
micro-burette with a capillary tip to 100, 250, or 500 mL of water in	sized); twice-distilled under reduced pressure; $d_4^{20}$ 0.9646,	
a narrow-mouthed stock bottle with a well-ground glass stopper. The	$n_{\rm D}^{20}$ 1.4368.	
bottle was shaken after each addi- tion of ester. 1-5 mg of Sudan IV	(2) Distilled.	
dye was put into the water to im- prove the end-point of the titra-	ESTIMATED ERROR:	
tion. At saturation, one additional drop of ester was sufficient to	Not specified.	
convert the floating rough indica- tor particles into dark transparent		
droplets.	DEEEDENCES.	
	1 Selected Values of Pronoution of	
	1. Selected values of Properties of Hydrocarbons and Related Com- pounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, <u>1973</u> .	

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<pre>COMPONENTS: (1) Phosphoric acid dibutyl methylphenyl ester (dibutyl tolyl phosphate); C<sub>15</sub>H<sub>25</sub>O<sub>4</sub>P; [26446-69-5] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Apelblat, A. <i>J. Chem. Soc.</i> B <u>1969</u> , 175-7.
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of water in phosphoric 25°C was reported to be 1.50 mol(2)/L mass/volume basis is 27.0 g(2)/L sln	acid dibutyl methylphenyl ester at sln. The corresponding value on a (compiler).

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The mixture was equilibrated by vigorous stirring for 30 min. and settling for 12 h. The organic phase was analyzed with the Karl Fischer reagent. Preliminary ex- periments showed that stirring and settling times were sufficient.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Synthesized at the Plastics    Research Laboratory of the    Weizmann Institute of Science;    used as received; b.p. 132-5°C    at 0.3 mm Hg, n<sup>5</sup><sub>D</sub> 1.4722. (2) Not specified.  ESTIMATED ERROR:    Temp. ±0.1°C.  REFERENCES: </pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) 1,2-Benzenedicarboxylic acid bis(2-methylpropyl) ester (diisobutyl phthalate); CorHerOr: [84=69=5]</pre>	Leyder, F.; Boulanger, P.	
	Bull. Environ. Contam. Toxicol. <u>1983</u> , 30(2), 152-7.	
(2) Water; H <sub>2</sub> O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
The solubility of 1,2-benzenedicarbox in water at 20°C was reported to be 7 0.0203 g(1)/L.	<pre>kylic acid bis(2-methylpropyl) ester 2.30 x 10<sup>-5</sup> mol(1)/L and</pre>	
ΔΙΙΥΤΙ.ΤΔΡΥ	τηξορμαφτον	
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The analytical method as described in the OECD Guidelines for Testing of Chemicals (ref 1) was used. Gas chromatography analyses were con- ducted on a Girdel 3000 FFLE ap- paratus with flame-ionization de- tection. A 4 mm x 180 m stainless steel column packed with 3% OV-1 on 80-100 mesh Chromosorb W-AW-DMCS and helium at a 20mL/min flow rate were used. Samples were fortified with an internal standard, extract- ed, and concentrated to 1 mL of hexane solution. "Solvent flush" and "hot needle" injection tech- niques were used. The two methods gave similar results. Peak heights were measured throughout. UV meas- urements were made by using 1-cm cells in a Perkin-Elmer model 552 uv-Visible spectrophotometer.	<ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) BASF "Palatinol IC"; used as received.</li> <li>(2) Deionized and distilled from KMnO<sub>4</sub>.</li> </ul>	
	ESTIMATED ERROR: Temp. ±1°C. REFERENCES: 1. OECD Guidelines for Testing of Chemicals, Paris, OECD, <u>1981</u> . (methods 101, 105).	

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COMPONENTS:	EVALUATOR:
<pre>(1) 1,2-Benzenedicarboxylic acid dibutyl ester (dibutyl phthalate); C<sub>16</sub>H<sub>22</sub>O<sub>4</sub>; [84-74-2]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H <sub>2</sub> O; [7732-18-5]	December, 1988

### CRITICAL EVALUATION:

Quantitative solubility data for the 1,2-benzenedicarboxylic acid dibutyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>TABLE 1: Quantitative Solubility Studies of the</u> <u>1,2-Benzenedicarboxylic acid dibutyl ester (1) - Water (2) System</u>			
Reference	T/K	Solubility	Method
Krupatkin and Glagoleva (ref 1)	298	mutual	titration
Schwarz (ref 2)	297 <sup>a</sup>	(1) in (2)	chromatographic
Leyder and Boulanger (ref 3)	293	(1) in (2)	GLC

<sup>a</sup> 23.5 °C.

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. SOLUBILITY OF 1,2-BENZENEDICARBOXYLIC ACID DIBUTYL ESTER (1) IN WATER (2)

All the available data for the solubility of 1,2-benzenedicarboxylic acid dibutyl ester (1) in water (2) are summarized in Table 2. The value of Krupatkin and Glagoleva (ref 1) is much higher than the other studies and is rejected. Pending further independent studies the remaining data (ref 2,3) must be regarded as very Tentative.

(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) 1,2-Benzenedicarboxylic acid dibutyl ester (dibutyl phthalate); C<sub>16</sub>H<sub>22</sub>O<sub>4</sub>; [84-74-2]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H <sub>2</sub> O; [7732-18-5]	December, 1988

CRITICAL EVALUATION: (continued)

### TABLE 2: Reported Solubilities of 1,2-Benzenedicarboxylic acid dibutyl ester (1) in Water (2)

T/K		Reported	Solubilities	
	10 <sup>3</sup> g(1)/100g sln			10 <sup>7</sup> x <sub>1</sub>
293	1.01 (ref 3)			6
297 <sup>a</sup>	1.83 (ref 2)			12
298	40 (ref 1) <sup>b</sup>			260 <sup>b</sup>

<sup>a</sup> 23.5 <sup>o</sup>C.

b Rejected value.

### 2. SOLUBILITY OF WATER (2) IN 1,2-BENZENEDICARBOXYLIC ACID DIBUTYL ESTER (1)

As the only available datum for the solubility of water (2) in 1,2benzenedicarboxylic acid dibutyl ester (1) is that of Krupatkin and Glagoleva (ref 1) no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental solubility but it may be noted that solubilities reported by these authors often differ from reliable values.

REFERENCES

1.	Krupatkin,	I.	L.;	Glagoleva,	М.	F.	Zh.	Prikl.	Khim.	<u>1972,</u>	45,	1317-
	20.											

- 2. Schwarz, F. P. Anal. Chem. <u>1980</u>, 52, 10-15.
- 3. Leyder, F.; Boulanger, P. Bull. Environ. Contam. Toxicol. <u>1983</u>, 30, 152-7.

COMPONENTS: (1) 1,2-Benzenedicarboxylic acid dibutyl ester (dibutyl phthalate); C <sub>16</sub> H <sub>22</sub> O <sub>4</sub> ; [84-74-2]	ORIGINAL MEASUREMENTS: Krupatkin, I.L.; Glagoleva, M.F. Zh. Prikl. Khim. <u>1972</u> , 45, 1317-20.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	Z. Maczynska
25°C was reported to be 0.04 g(1)/100 tion, $x_1$ , value calculated by the con The solubility of water in 1,2-benzed 25°C was reported to be 0.62 g(2)/100 tion, $x_2$ , value calculated by the con	Og sln. The corresponding mole frac- mpiler is 3x10 <sup>-5</sup> . nedicarboxylic acid dibutyl ester at Og sln. The corresponding mole frac- mpiler is 0.088.
AUXTLIARY	TNFORMATION
	SOURCE AND DURITY OF MATERIALS.
METHOD/APPARATUS/PROCEDURE: The titration method was used. The measurements were carried out in a water thermostat. The data were reported together with the ternary system 1,2-benzenedicarboxylic acid dibutyl ester-water-2-furancarbonal (dibutyl phthalate-water-furfural). No further details were reported in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified; b.p. 340°C, d<sup>25</sup> 1.0485, n<sup>25</sup> 1.4882. (2) Twice distilled.  ESTIMATED ERROR: Temp. ±0.1°C. </pre>

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<pre>COMPONENTS: (1) 1,2-Benzenedicarboxylic acid dibutyl ester (dibutyl phthalate); C<sub>16</sub>H<sub>22</sub>O<sub>4</sub>; [84-74-2] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Schwarz, F.P. <i>Anal. Chem.</i> <u>1980</u> , 52, 10-5.
VARIABLES: T/K = 297	PREPARED BY: A. Skrzecz
EXPERIMENTAL VALUES: The solubility of 1,2-benzenedicarbox 23.5°C was reported to be 0.00183 g(1 fraction, $x_1$ , value calculated by the	xylic acid dibutyl ester in water at .)/100g sln. The corresponding mole a compiler is 1.18 x 10 <sup>-6</sup> .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The elution chromatographic method was used. The column was filled with Chromosorb P (80-120 mesh, 4-6 m <sup>2</sup> /g by BET) coated with the solute and prepared in a special way as described in the paper. The water passing through the sol- ute column was collected in gradu- ated vessels. The measurements were initiated after the appearance of the solute depleted light pink col- ored zone (solvent zone) on Chromo- sorb P. Each measurement consisted of turning off the flow, measuring the length of the zone and the to- tal volume of the water passed through the column. Measurements were initiated after the solvent zone extended 0.3 cm down the length of the column and were continued until the solvent zone extended down at least 25% of the column length.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, reagent grade; used as received; d<sup>20</sup> 1.047. (2) Distilled.  ESTIMATED ERROR: Temp. ±1.5°C. Soly. ±0.00006 g(1)/100g sln (standard deviation).  REFERENCES: </pre>

<pre>(2) Water; H<sub>2</sub>O; [7732-18-5] VARIABLES: T/K = 293</pre>	PREPARED BY:		
<pre>(1) 1,2-Benzenedicarboxylic acid dibutyl ester (dibutyl phthalate); C<sub>16</sub>H<sub>22</sub>O<sub>4</sub>; [84-74-2]</pre>	Leyder, F.; Boulanger, P. Bull. Environ. Contam. Toxicol. <u>1983</u> , 30(2), 152-7.		
COMPONENTS:	ORIGINAL MEASUREMENTS:		

EXPERIMENTAL VALUES:

The solubility of 1,2-benzenedicarboxylic acid dibutyl ester in water at  $20^{\circ}$ C was reported to be 3.63 x  $10^{-5}$  mol(1)/L and 0.0101 g(1)/L.

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The analytical method as described in the OECD Guidelines for Testing of Chemicals (ref 1) was used. Gas chromatography analyses were conducted on a Girdel 3000 FFLE apparatus with flame-ionization detection. A 4 mm x 180 m stainless steel column packed with 3% OV-1 on 80-100 mesh Chromosorb W-AW-DMCS and helium at a 20mL/min flow rate were used. Samples were fortified with an internal standard, extracted, and concentrated to 1 mL of hexane solution. "Solvent flush" and "hot needle" injection tech-niques were used. The two methods gave similar results. Peak heights were measured throughout. UV measurements were made by using 1-cm cells in a Perkin-Elmer model 552 uv-Visible spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

- Fluka; purity >98%; used as received.
- (2) Deionized and distilled from KMnO<sub>4</sub>.

ESTIMATED ERROR:

Temp. ±1°C.

### **REFERENCES:**

1. OECD Guidelines for Testing of Chemicals, Paris, OECD, <u>1981</u>. (methods 101, 105).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phosphoric acid butyl	Apelblat, A.
bis(methylphenyl) ester	J. Chem. Soc. B <u>1969</u> , 175-7.
$C_{18}H_{23}O_{4}P;$ [25657-10-7]	
(2) Water; $H_2O$ ; [7732-18-5]	
(-,	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of water in phosphoric at 25°C was reported to be 0.69 mol(2 a mass/volume basis is 12.4 g(2)/L sl The density of the ester-phase was re	acid butyl bis(methylphenyl) ester )/L sln. The corresponding value on .n (compiler). eported to be $d^{25}$ 1.1097.
AUXILIARY 1	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The mixture was equilibrated by vigor- ous stirring for 30 min. and settl- ing for 12 h. The organic phase was analyzed with the Karl Fischer rea- gent. Preliminary experiments show- ed that stirring and settling times were sufficient.	<ul> <li>(1) Synthesized at the Plastics Research Laboratory of the Weizmann Institute of Science; used as received; b.p. 180°C at 0.25 mm Hg, d<sub>4</sub><sup>25</sup> 1.1118, n<sub>D</sub><sup>25</sup> 1.5160.</li> <li>(2) Not specified.</li> <li>ESTIMATED ERROR: Temp. ±0.1°C.</li> </ul>
	REFERENCES:

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ORIGINAL MEASUREMENTS: Leyder, F.; Boulanger, P. Bull. Environ. Contam. Toxicol. <u>1983</u> , 30(2), 152-7.
PREPARED BY:
A. Skrzecz
xylic acid dipentyl ester in water at 2.6 x 10 <sup>-6 b</sup> mol(1)/L and 0.0001 <sup>a</sup> ,
INFORMATION
<pre>SOURCE AND PURITY OF MATERIALS: (1) Kodak, practical grade; purity &gt;90%; used as received. (2) Deionized and distilled from KMnO<sub>4</sub>. ESTIMATED ERROR: Temp. ±1°C. REFERENCES: 1. OECD Guidelines for Testing of Chemicals, Paris, OECD, <u>1981</u>. (methods 101, 105).</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phosphoric acid	Apelblat, A.
tris(butoxyethyl) ester	J. Chem. Soc. B 1969, 175-7.
(tri(butoxyetnyi) phosphate);	
$C_{18}R_{39}O_7P;$ [78-51-5]	
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of water in phosphoric was reported to be 4.26 mol(2)/L sln mass/volume basis is 76.7 g(2)/L sln The density of the ester-phase was re	c acid tris(butoxyethyl) ester at 25°C . The corresponding value on a (compiler). aported to be $d^{25}$ 1.0204.
AIIXTLTARY	TNFORMATTON
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The mixture was equilibrated by vigor- ous stirring for 30 min. and settl- ing for 12 h. The organic phase was analyzed with the Karl Fischer rea- gent. Preliminary experiments show- ed that stirring and settling times were sufficient.	<ul> <li>(1) Albright and Wilson Co; purified by method described by Alcock, Grimley, Healy, Kennedy and McKay (ref 1); d<sub>4</sub><sup>25</sup> 1.0181, n<sub>D</sub><sup>25</sup> 1.4358.</li> <li>(2) Not specified.</li> </ul>
	ESTIMATED ERROR:
	Temp. ±0.1 <sup>°</sup> C.
	DEEDENCES.
	KEFEKENCES:
	<ol> <li>Alcock, K.; Grimley, S.S.; Healy, T.V.; Kennedy, J.; McKay, H.A.C. Trans. Faraday Soc. <u>1956</u>, 52, 39.</li> </ol>

### CRITICAL EVALUATION:

Quantitative solubility data for the 1,2-benzenedicarboxylic acid butyl phenylmethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>TABLE 1: Quantitative Solubility Studies of the</u> <u>1,2-Benzenedicarboxylic acid butyl phenylmethyl ester (1) -</u> <u>Water (2) System</u>				
Reference	T/K	Solubility	Method	
Krupatkin and Glagoleva (ref 1)	298	mutual	titration	
Leyder and Boulanger (ref 2)	293	(1) in (2)	GLC	

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.

#### SOLUBILITY OF 1,2-BENZENEDICARBOXYLIC ACID BUTYL PHENYLMETHYL 1. ESTER (1) IN WATER (2)

All the available data for the solubility of 1,2-benzenedicarboxylic acid butyl phenylmethyl ester (1) in water (2) are summarized in Table 2. The data are in serious disagreement differing by three orders of magnitude! The more recent value of Leyder and Boulanger (ref 2) using a more appropriate technique is probably more reasonable but, in the absence of further studies, it is not possible to reject the datum of Krupatkin and Glagoleva (ref 1).

<u>of 1,2-Ber</u>	nzenedicarboxylic acid butyl phenylmethy	<u>l ester (1) in Water (2</u>
T/K	Reported Sol	lubilities
	10 <sup>4</sup> g(1)/100g sln	10 <sup>7</sup> x <sub>1</sub>
293	2.82 <sup>ª</sup> (ref 2)	1.63 <sup>a</sup>
298	2100 <sup>b</sup> (ref 1)	1200 <sup>b</sup>

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Unlikely value, see text.

(continued next page)

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COMP((1))	ONENTS: 1,2-Benzenedicarboxylic acid butyl phenylmethyl ester (butyl benzyl phthalate); C <sub>19</sub> H <sub>20</sub> O <sub>4</sub> ; [85-68-7] 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 December, 1988
CRIT	ICAL EVALUATION: (continued)	
2. benzo and o inter solu autho	SOLUBILITY OF WATER (2) IN 1,2-BE PHENYLMETHYL EST The only available datum for the enedicarboxylic acid butyl phenylm Glagoleva (ref 1) and thus no Crit rested user is referred to the rel bility but it should be noted that ors often differ from reliable val	NZENEDICARBOXYLIC ACID BUTYL FER (1) solubility of water (2) in 1,2- ethyl ester (1) is that of Krupatkin ical Evaluation is possible. The evant Data Sheet for the experimental solubilities reported by these ues in well characterized systems.
REFEI	RENCES	
1.	Krupatkin, I. L.; Glagoleva, M. 1795-9.	F. Zh. Prikl. Khim. <u>1972</u> , 45,
2.	Leyder, F.; Boulanger, P. Bull. 152-7.	Environ. Contam. Toxicol. <u>1983</u> , 30,

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Benzenedicarboxylic acid	Krupatkin, I.L.; Glagoleva, M.F. Zh. Prikl. Khim. 1972, 45, 1795-9
(butyl benzyl phthalate);	211. 111. (11. 11. 11. 11. 11. 11. 11. 11
$C_{19}H_{20}O_4$ ; [85-68-7]	
(2) Water: $H_{2}O$ : [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES:	
The solubility of 1,2-benzenedicarbox	ylic acid butyl phenylmethyl ester in
water at 25°C was reported to be 0.21	g(1)/100g sln. The corresponding
mole fraction, $x_1$ , value calculated k	by the compiler is 1.21 x $10^{-4}$ .
The solubility of water in 1,2-benzer	hedicarboxylic acid butyl phenylmethyl
ester at 25°C was reported to be 0.07 mole fraction, $x_{\rm e}$ , value calculated h	g(2)/100g sin. The corresponding
AUXILIARY	
	SOURCE AND PURTTY OF MATERIALS:
	SOURCE AND FORTH OF MATERIALS.
The titration method was used as given by Krupatkin and Glagoleva	(1) Source not specified; b.p.236°C, $d_{25}^{25}$ 1.1065,
(ref 1). The samples were titrated up to turbidity. The data were re- ported together with the ternary	$n_{\rm D}^{25}$ 1.5180.
	(2) Twice distilled.
system 1,2-benzenedicarboxylic acid butyl phenylmethyl ester-water-	
2-furancarbonal (butyl benzyl	
phthalate-water-furfural). No further details were reported in the paper.	ESTIMATED ERROR:
	Not specified.
	REFERENCES:
	1. Krupatkin, T.L.: Glagoleva, M.F.
	Zh. Prikl. Khim. <u>1969</u> , 42, 880.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-BenzenealCarpoxy11C acid	Leyder, F.; Boulanger, P.
(buty) benzyl phthalate):	Bull. Environ. Contam. Toxicol.
$C_{10}H_{20}O_{4}$ ; [85-68-7]	<u>1983</u> , 30(2), 152-7.
(2) Water: $H \cap [7722-19-5]$	
(2) water; $H_20$ ; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
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The solubility of 1,2-benzenedicarboxylic acid butyl phenylmethyl ester in water at 20°C was reported to be 9.02 x 10 <sup>-6</sup> mol(1)/L and 0.00282 g(1)/L.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method as described in the OECD Guidelines for Testing of Chemicals (ref 1) was used. Gas chromatography analyses were con- ducted on a Girdel 3000 FFLE ap- paratus with flame-ionization de- tection. A 4 mm x 180 m stainless steel column packed with 3% 0V-1 on	(1) Bayer Unimoll BB; purity not specified; used as received.
	(2) Deionized and distilled from KMnO <sub>4</sub> .
80-100 mesh Chromosorb W-AW-DMCS	ESTIMATED ERROR:
were used. Samples were fortified	
with an internal standard, extract-	Temp. ±1°C.
hexane solution. "Solvent flush"	
and "hot needle" injection tech- niques were used. The two methods	
gave similar results. Peak heights	REFERENCES:
urements were made by using 1-cm	1. OECD Guidelines for Testing of
cells in a Perkin-Elmer model 552 uv-Visible spectrophotometer.	Chemicals, Paris, OECD, <u>1981</u> . (methods 101, 105).

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Benzenedicarboxylic acid	Krupatkin, I.L.; Glagoleva, M.F.
(butyl octyl phthalate):	211. FIIKI. KIIM. <u>1972</u> , 45, 1795-9.
$C_{20}H_{30}O_4$ ; [84-78-6]	
(2) Water: $H_0$ (7732-18-5)	
$(2)$ water, $n_20$ , $[7732-10-5]$	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
The solubility of 1,2-benzenedicarbox at 25°C was reported to be 0.04 g(1)/ fraction, $x_1$ , value calculated by the The solubility of water in 1,2-benzer at 25°C was reported to be 0.02 g(2)/ fraction, $x_2$ , value calculated by the	kylic acid butyl octyl ester in water (100g sln. The corresponding mole a compiler is 2.2 x 10 <sup>-5</sup> . medicarboxylic acid butyl octyl ester (100g sln. The corresponding mole a compiler is 0.0037.
AUXILIARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used as given by Krupatkin and Glagoleva	(1) Source not specified; $d_{25}^{25}$ 1.0097, $n_{\rm D}^{25}$ 1.4868.
(ref 1). The samples were titrated up to turbidity. The data were re- ported together with the ternary system 1,2-benzenedicarboxylic acid butyl octyl ester-water-2-furan- carbonal (butyl octyl phthalate- water-furfural). No further details were reported in the paper.	(2) Twice distilled.
	ESTIMATED ERROR:
	Not specified.
	KEFERENCES:
	<ol> <li>Krupatkin, I.L.; Glagoleva, M.F. Zh. Prikl. Khim. <u>1969</u>, 42, 880.</li> </ol>

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) L-Ascorbic acid	Swern, D.
6-hexadecanoate	J Am Chom Soc 1949 71 3256
(L-ascorbyl palmitate);	$5. \text{ Am}. \text{ chem}. \text{ 50c}. \frac{1343}{1343}, 71, 3230.$
$C_{22}H_{38}O_7; [137-66-6]$	
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
<pre>EXPERIMENTAL VALUES: The solubility of L-ascorbic acid 6-H reported to be 0.56 g(1)/100g<sup>a,b</sup> and mass per cent and mole fractions, x<sub>1</sub>, are 0.56 g(1)/100g sln, 0.31 g(1)/100 The units g(1)/100g were reported as</pre>	hexadecanoate in water at 25°C was 0.31 g(1)/100g <sup>a,c</sup> . The corresponding values calculated by the compiler og sln and 2.4 x 10 <sup>-4</sup> , 1.4 x 10 <sup>-4</sup> . above.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDUPE •	SOURCE AND PURTTY OF MATERIALS.
The analytical methods were used	(1) Not specified
An excess of ester was shaken with	
water until an equilibrium was obtained. The dissolved ester was determined both by titration with 0.1 N NaOH and by evaporation of water. At least two determinations	(2) Not specified.
were made.	
	Temp. ±0.10°C. Soly. ±0.5% (precision of duplicates).
	REFERENCES:

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<pre>COMPONENTS: (1) 1,2-Benzenedicarboxylic acid     bis(2-ethylhexyl) ester     (bis(2-ethylhexyl) phthalate);     C<sub>24</sub>H<sub>38</sub>O<sub>4</sub>; [117-81-7] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Leyder, F.; Boulanger, P. Bull. Environ. Contam. Toxicol. <u>1983</u> , 30(2), 152-7.
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of 1,2-benzenedicarboxylic acid bis(2-ethylhexyl) ester in water at 20°C was reported to be 1.05 x 10 <sup>-7</sup> mol(1)/L and 4.1 x 10 <sup>-5</sup> g(1)/L.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method as described in the OECD Guidelines for Testing of Chemicals (ref 1) was used. Gas chromatography analyses were con- ducted on a Girdel 3000 FFLE ap- paratus with flame-ionization de- tection. A 4 mm x 180 m stainless steel column packed with 3% OV-1 on 80-100 mesh Chromosorb W-AW-DMCS and helium at a 20mL/min flow rate were used. Samples were fortified with an internal standard, extract- ed, and concentrated to 1 mL of hexane solution. "Solvent flush" and "hot needle" injection tech- niques were used. The two methods gave similar results. Peak heights were measured throughout. UV meas- urements were made by using 1-cm cells in a Perkin-Elmer model 552 uv-Visible spectrophotometer.	<ul> <li>(1) Essochem DOP; purity not specified; used as received.</li> <li>(2) Deionized and distilled from KMnO<sub>4</sub>.</li> <li>ESTIMATED ERROR: Temp. ±1°C.</li> <li>REFERENCES:</li> <li>1. OECD Guidelines for Testing of Chemicals, Paris, OECD, <u>1981</u>. (methods 101, 105).</li> </ul>

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<pre>COMPONENTS: (1) Phosphoric acid tris(2-ethylhexyl) ester (tri(2-ethylhexyl) phosphate); C<sub>24</sub>H<sub>51</sub>O<sub>4</sub>P; [78-42-2] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Apelblat, A. <i>J. Chem. Soc.</i> B <u>1969</u> , 175-7.
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of water in phosphoric 25°C was reported to be 0.81 mol(2)/I mass/volume basis is 14.6 g(2)/L sln The density of the ester-phase was re	c acid tris(2-ethylhexyl) ester at c sln. The corresponding value on a (compiler). aported to be $d^{25}$ 0.9235.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The mixture was equilibrated by vigorous stirring for 30 min. and settling for 12 h. The organic phase was analyzed with the Karl Fischer reagent. Preliminary ex- periments showed that stirring and settling times were sufficient.	<ul> <li>(1) Albright and Wilson Co; purified by method described by Alcock, Grimley, Healy, Kennedy and McKay (ref 1); d<sub>4</sub><sup>25</sup> 0.9220, n<sub>D</sub><sup>25</sup> 1.4417.</li> <li>(2) Not specified.</li> <li>ESTIMATED ERROR: Temp. ±0.1°C.</li> </ul>
	REFERENCES:
	<pre>1. Alcock, K.; Grimley, S.S.; Healy, T.V.; Kennedy, J.; McKay, H.A.C. Trans. Faraday Soc. 1956, 52, 39.</pre>

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Benzenedicarboxylic acid	Krupatkin, I.L.; Glagoleva, M.F.
dinonyl ester	Zh. Prikl. Khim. 1972. 45
(dinonyl phthalate);	1317-20.
$C_{26}H_{42}O_4; [84-76-4]$	
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	Z. Maczynska
EXPERIMENTAL VALUES: The solubility of 1,2-benzenedicarbox 25°C was reported to be 0.02 g(1)/100 tion, $x_1$ , value calculated by the com The solubility of water in 1,2-benzen 25°C was reported to be 0.09 g(2)/100 tion, $x_2$ , value calculated by the com	kylic acid dinonyl ester in water at og sln. The corresponding mole frac- mpiler is 9 x 10 <sup>-6</sup> . Medicarboxylic acid dinonyl ester at og sln. The corresponding mole frac- mpiler is 0.02.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The titration method was used. The measurements were carried out in a water thermostat. The data were re- ported together with the ternary system 1,2-benzenedicarboxylic acid dinonyl ester-water-2-furancarbonal (dinonyl phthalate-water-furfural). No further details were reported in the paper.	(1) Source not specified; b.p. 240°C, $d_4^{25}$ 0.9819, $n_D^{25}$ 1.4852. (2) Twice distilled.
	ESTIMATED ERROR:
	Temp. ±0.1°C.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzoic acid, 2-hydroxy-,	Seidell, A.
cinchonan-9-ol,	Hygienic Lab. Bull. <u>1910</u> , No. 67,
(quinine salicylate);	98 pp (US Govt. Printing Office,
C <sub>27</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub> ; [750-90-3]	Washington DC)
(2) Water: $H_2O$ ; [7732-18-5]	
	DEFDARED BV.
17K = 298	G.T. heller
The solubility of 2-hydroxybenzoic ac ester in water at 25°C was reported t sponding mole fraction, $x_1$ , value cal	cid 6'-methoxycinchonan-9-ol (8α,9R) to be 0.065 g(1)/100g sln. The corre- culated by the compiler is 2.5 x 10 <sup>-5</sup> .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used.	(1) Merck, m.p. ca. 195 <sup>0</sup> C.
Appropriate quantities of (1) and (2) were shaken together. The a-	(2) Distilled (no details given).
mount of dissolved (1) was deter- mined by evaporation of a known quantity of the saturated solu-	
constant weight in a vacuum desic-	
cator.	ESTIMATED ERROR:
	Temp. not stated. Soly. not stated.
	REFERENCES:

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COMPONENTS: (1) 1,2-Benzenedicarboxylic acid	ORIGINAL MEASUREMENTS: Krupatkin, I.L.; Glagoleva, M.F.
(didodecyl ester (didodecyl phthalate); C <sub>32</sub> H <sub>54</sub> O <sub>4</sub> ; [2432-90-8]	Zh. Prikl. Khim. <u>1972</u> , 45, 1317-20.
(2) Water; H <sub>2</sub> O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	Z. Maczynska
EXPERIMENTAL VALUES: The solubility of 1,2-benzenedicarboxylic acid didodecyl ester in water at $25^{\circ}$ C was reported to be 0.07 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calculated by the compiler is 3 x $10^{-5}$ . The solubility of water in 1,2-benzenedicarboxylic acid didodecyl ester at $25^{\circ}$ C was reported to be 0.02 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calculated by the compiler is 0.006.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. The measurements were carried out in a water thermostat. The data were re- ported together with the ternary system 1,2-benzenedicarboxylic acid didodecyl ester-water-2-furan- carbonal (didodecyl phthalate-	(1) Source not specified; $d_4^{25}$ 0.9548, $n_D^{25}$ 1.4839.
	(2) Twice distilled.
were reported in the paper.	ESTIMATED ERROR:
	Temp. ±0.1°C.
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