

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.
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CRITICAL EVALUATION: (continued)

As indicated in the footnotes to Table 1, quantitative solubility data for heptane in D_2O (ref 7) are available. However, as no comparable data have been reported no critical evaluation of the reliability of these data can be made. The interested user is referred to the relevant data sheets.

In the heptane-water system the mutual solubilities are sufficiently low to enable data reported in w/v fractions (or equivalent) to be converted to mass percent solubilities with reasonable precision by assuming solution densities to be the same as the pure solvents. These conversions are made on the Data Sheets and the data so obtained are included in this Evaluation. For convenience, further discussion of this system will be divided into three parts.

In the Tables which follow, values obtained by the Evaluator by graphical interpolation or extrapolation of the original measurements in the Data Sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits.

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

The extremely low solubility of heptane in water presents a daunting analytical problem. Nevertheless, all the modern investigations (ref 12, 13, 15, 16, 18), employing GLC, are in good agreement. The older studies, by Fuhner (ref 1), Durand (ref 5) and Guseva and Parnov (ref 7), and the more recent measurements of Budantseva *et al.* (ref 17) and Korenman and Aref'eva (ref 19), are an order of magnitude higher than the GLC results and are therefore rejected. The value of Bittrich *et al.* (ref 21) at an unspecified temperature and the order of magnitude data of Booth and Everson (ref 4) and McCants *et al.* (ref 6) are also rejected. All other data are included in Table 2 except for the value of Krzyzanowska and Szeliga (ref 20) which does not appear to be independent of that of Price (ref 18) and has therefore been excluded from consideration.

Selected data from Table 2 are also plotted in Figure 1 which emphasises the general agreement between the various independent studies. Application of the van't Hoff equation to the data in Table 2 gives $\Delta H_{sln}^\infty = -2.43 \text{ kJ mol}^{-1}$ and $\Delta C_p^\infty, sln = 472 \text{ JK}^{-1} \text{ mol}^{-1}$ which are similar to calorimetric values reported for closely related hydrocarbons (ref 24).

(continued next page)

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A. Australia. October 1986.
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CRITICAL EVALUATION: (continued)

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

T/K	Solubility Values		
	Reported values $10^4 g(1)/100g\ sln$	"Best" values ($\pm \sigma_n$) $10^4 g(1)/100g\ sln$	$10^7 x_1$
273	1.9* (ref 13), 4.39 (ref 16)	3 ± 1	5
283	2.0* (ref 13)	2.0	3.6
293	2.3* (ref 13), 2.57 (ref 23)	2.4 ± 0.2	4.3
298	2.93 (ref 12), 2.66 (ref 13), 2.8 (ref 15), 3.37 (ref 16), 2.24 (ref 18), 2.9 (ref 22), 2.51 (ref 23)	2.4 ± 0.2	4.3
303	2.2* (ref 13), 2.36* (ref 18), 2.49 (ref 23)	2.4 ± 0.1	4.1
313	2.3* (ref 13), 2.62 (ref 18)	2.5 ± 0.2	4.5
323	2.93* (ref 18)	2.9	5.2
333	3.3* (ref 18)	3.3	5.9
363	3.9* (ref 18)	3.9	7.0
373	5.8* (ref 18)	5.8	10
393	13* (ref 18)	13	23
413	31* (ref 18)	31	56

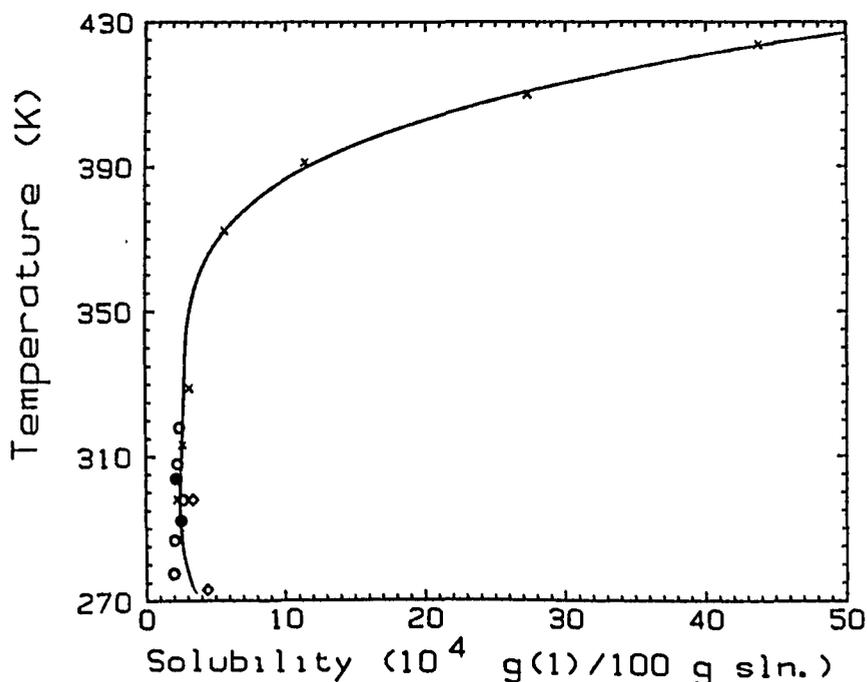


FIGURE 1. Solubility of heptane in water; selected data: ref 13 (\circ); ref 16 (\diamond); ref 18 (\times), ref 23 (\bullet).

(continued next page)

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A. Australia. October 1986.
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CRITICAL EVALUATION: (continued)

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

In spite of the analytical difficulty of accurate determination of the low concentrations involved, the various reported values of the solubility of water in heptane are in reasonable agreement. However, the amount of data available is much smaller than for heptane in H₂O.

The values of Black *et al.* (ref 3), the higher temperature ($T > 293\text{K}$) data of Englin *et al.* (ref 9) and the value of Zelvenskii *et al.* (ref 10) are higher than other studies (ref 8,14,16,17,21) and are therefore rejected. All other values are listed in Table 3.

TABLE 3: Tentative Values of the Solubility
of Water (2) in Heptane (1)

T/K	Solubility Values		
	Reported values 10 ³ g(2)/100 g sln	"Best" values ($\pm \sigma_n$) ^a 10 ³ g(2)/100 g sln	10 ⁴ x ₂
273	2.7 (ref 9), 2.6 (ref 16)	2.7	1.5
283	5.4 (ref 9)	5.4	3.0
293 ^b	9.6 (ref 9), 9 (ref 17)	9	5.0
298	9.1 (ref 8), 8.2 (ref 16), 12.1 (ref 21)	10 \pm 2	5.6
313	13 (ref 17), 15.6 (ref 21)	14	7.8

^a Because of the limited amount of data at temperatures other than 298K, σ_n values would be misleading and have therefore not been calculated.

^b A value of 5.73×10^{-3} g(2)/100 g sln reported at 295.7K in ref 14.

The data in Table 3 are also plotted in Figure 2. Application of the van't Hoff equation to the "Best" values of Table 3 gives $\Delta H_{\text{sln}}^{\infty} = 23 \text{ kJ mol}^{-1}$ and $\Delta C_{\text{p,sln}}^{\infty} = -1050 \text{ JK}^{-1} \text{ mol}^{-1}$. Whilst the $\Delta H_{\text{sln}}^{\infty}$ is reasonable by comparison with related systems (e.g. water in hexane), $\Delta C_{\text{p,sln}}^{\infty}$ values for the dissolution of water in hydrocarbons are normally ca. $+100 \text{ JK}^{-1} \text{ mol}^{-1}$. This is evidenced by a general flattening off for the solubility-temperature curve at higher temperatures (e.g. water in hexane or benzene) rather than the apparent increasing gradient seen in Figure 2. That is, the reported solubilities at higher temperatures are probably too low.

(continued next page)

COMPONENTS:

- (1) Heptane; C_7H_{16} ; [142-82-5]
 (2) Water; H_2O ; [7732-18-5]

EVALUATOR:

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 C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia.

October 1986.

CRITICAL EVALUATION: (continued)

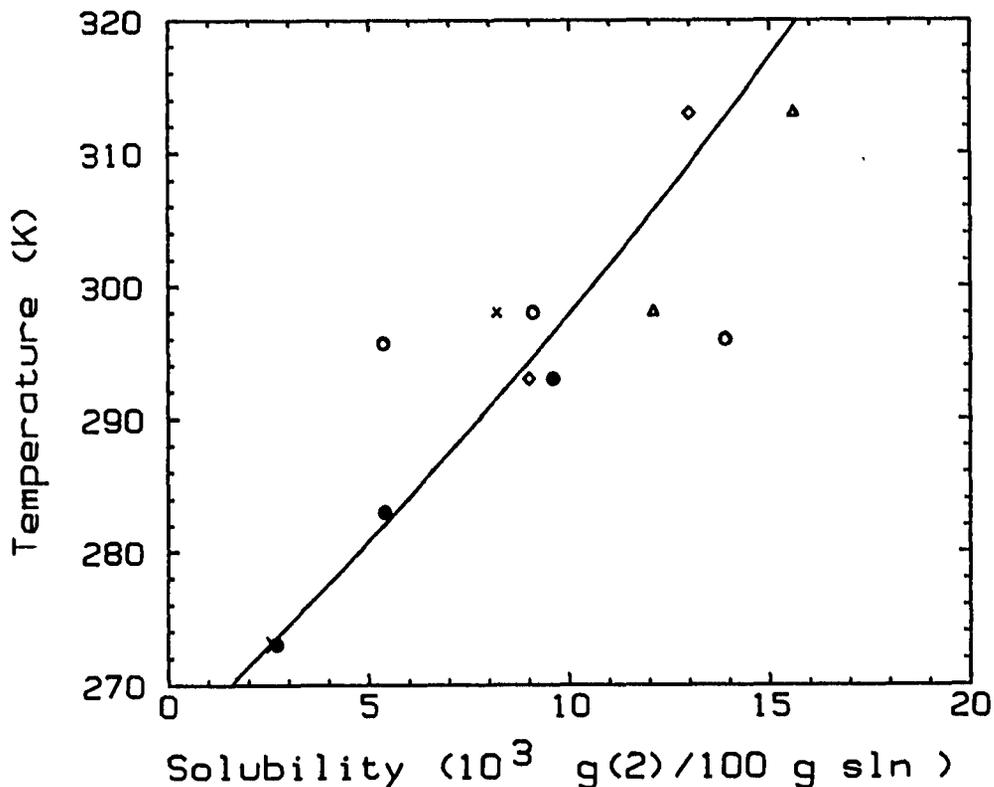


FIGURE 2. Solubility of water in heptane: ref 9 (●); ref 16 (x); ref 17 (◇); ref 21 (Δ); other data (○). Full line represents curve of best fit.

3. SOLUBILITY STUDIES OF THE HEPTANE (1) - WATER (2) SYSTEM AT ELEVATED PRESSURES

The phase behaviour type of this system is topographically similar to that of benzene + water.

Solubility studies on the heptane + water system at pressures higher than atmospheric are listed in Table 4. The solubility data obtained by Guseva and Parnov (ref 7) are considerably greater than that obtained by Price (ref 18) under comparable conditions. In the absence of further independent studies it is not possible to prefer either data set and the interested user is referred to the relevant Data Sheets for experimental values. Meaningful comparisons with the data of other workers is also precluded because of the differences in conditions.

(continued next page)

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-83-5] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. October 1986.
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CRITICAL EVALUATION: (continued)

TABLE 4. Solubility Studies of the Heptane + Water System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Guseva and Parnov (ref 7)	along 3-phase line	345-460	(1) in (2)
Connolly (ref 11)	17-55	568-628	(1) in (2)
Price (ref 18)	along 3-phase line	295-424	(1) in (2)
Bröllos <i>et al.</i> (ref 25)	- ^a	- ^a	- ^a
Roof (ref 26)	6.3 ^b	519.0 ^b	- ^b

^a Qualitative statements and graph of phase behaviour only.

^b Critical point of unknown composition.

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- Zel'venskii, Ya.D.; Efremov, A.A.; Larin, G.M. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 3-7.
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<p>COMPONENTS:</p> <p>(1) Heptane; C₇H₁₆; [142-82-5]</p> <p>(2) Water; H₂O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.</p> <p>October 1986.</p>
<p>CRITICAL EVALUATION: (continued)</p> <p>REFERENCES (continued)</p> <p>18. Price, L.C. <i>Am. Assoc. Petrol. Geol. Bull.</i> <u>1976</u>, <i>60</i>, 213-44.</p> <p>19. Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, <u>1977</u>, .04.05.</p> <p>20. Krzyzanowska, T.; Szeliga, J. <i>Nafta (Katowice)</i> <u>1978</u>, <i>34</i>, 413-7.</p> <p>21. Bittrich, H.J.; Gedan, H.; Feix, G. <i>Z. Phys. Chem. Leipzig</i> <u>1979</u>, <i>260</i>, 1009-13.</p> <p>22. Rudakov, E.S.; Lutsyk, A.I. <i>Zh. Fiz. Khim.</i> <u>1979</u>, <i>53</i>, 1298-1300.</p> <p>23. Jonsson, J.A.; Vejrosta, J.; Novak, J. <i>Fluid Phase Equil.</i> <u>1982</u>, <i>9</i>, 279-86.</p> <p>24. Gill, S.J.; Nichols, N.F.; Wadso, I. <i>J. Chem. Thermodyn.</i> <u>1976</u>, <i>8</i>, 445-52.</p> <p>25. Bröllos, K.; Peter, K.; Schneider, G.M. <i>Ber. Bunsenges.</i> <u>1970</u>, <i>74</i>, 682-6.</p> <p>26. Roof, J.G. <i>J. Chem. Eng. Data</i> <u>1970</u>, <i>15</i>, 301-3.</p> <p>ACKNOWLEDGEMENTS</p> <p>The Evaluator thanks Dr Brian Clare for the regression analyses and graphics and Dr Marie-Claire Saulait-Pirson for comments and a preliminary draft of the reference list. Section 3 was written jointly with C. L. Young, Department of Physical Chemistry, University of Melbourne, Australia.</p>	

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Fühner, H. <i>Ber. Dtsch. Chem. Ges.</i> <u>1924</u> , 57, 510-5.
VARIABLES: One temperature: 15.5°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of heptane in water at 15.5°C was reported to be 0.007 mL(1)/100 mL sln or 0.005 g(1)/100 g sln.</p> <p>The corresponding mole fraction, x_1, calculated by the compiler is 0.9×10^{-5}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: In a stoppered measuring cylinder pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100 or 1000 cm ³ of (2) until a completely clear solution was obtained at the experimental temperature.	SOURCE AND PURITY OF MATERIALS: (1) source not specified; commercial grade; used as received. (2) not specified.
ESTIMATED ERROR: not specified.	
REFERENCES:	

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Black, C.; Joris, G.G.; Taylor, H.S. <i>J. Chem. Phys.</i> <u>1948</u> , <i>16</i> , 537-43.																				
VARIABLES: Temperature: 10-25°C	PREPARED BY: M.C. Haulait-Pirson																				
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in heptane at a total saturation pressure of 1 atm</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;"><u>t/°C</u></th> <th style="text-align: center;"><u>g(2)/100 g(1)</u></th> <th style="text-align: center;"><u>g(2)/100 g sln (compiler)</u></th> <th style="text-align: center;"><u>10⁴x₂ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td>10</td> <td style="text-align: center;">0.0077</td> <td style="text-align: center;">0.0077</td> <td style="text-align: center;">4.28</td> </tr> <tr> <td>20</td> <td style="text-align: center;">0.0136</td> <td style="text-align: center;">0.0136</td> <td style="text-align: center;">7.56</td> </tr> <tr> <td>20</td> <td style="text-align: center;">0.0126</td> <td style="text-align: center;">0.0126</td> <td style="text-align: center;">7.00</td> </tr> <tr> <td>25</td> <td style="text-align: center;">0.0151</td> <td style="text-align: center;">0.0151</td> <td style="text-align: center;">8.39</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>g(2)/100 g(1)</u>	<u>g(2)/100 g sln (compiler)</u>	<u>10⁴x₂ (compiler)</u>	10	0.0077	0.0077	4.28	20	0.0136	0.0136	7.56	20	0.0126	0.0126	7.00	25	0.0151	0.0151	8.39
<u>t/°C</u>	<u>g(2)/100 g(1)</u>	<u>g(2)/100 g sln (compiler)</u>	<u>10⁴x₂ (compiler)</u>																		
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25	0.0151	0.0151	8.39																		
AUXILIARY INFORMATION																					
METHOD/APPARATUS/PROCEDURE: <p>The method described in ref 1 in which tritium oxide acts as a tracer, was used. Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred in the counter through equilibration with ethanol vapor.</p>	SOURCE AND PURITY OF MATERIALS: (1) Ohio State University under an American Petroleum Institute project; purity not specified; used as received. (2) not specified.																				
ESTIMATED ERROR: soly. a few percent (type of error not specified).																					
REFERENCES: 1. Joris, G.G.; Taylor, H.S. <i>J. Chem. Phys.</i> <u>1948</u> , <i>16</i> , 45.																					

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (1) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Booth, H.S.· Everson, H.E. <i>Ind. Eng. Chem.</i> <u>1948</u> , 40, 1941-3.
VARIABLES: One temperature: 25.0°C (298.2 K)	PREPARED BY: G.T. Hefter
EXPERIMENTAL VALUES: <p>The solubility of <i>n</i>-heptane in water at 25.0°C was reported to be <0.04 mL (1)/100 mL (2). A similar request was reported for (1) in 40.0% (w/w?) aqueous sodium xylenesulfonate.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.02 mL. An excess of solute was added and the mixture allowed to come to equilibrium in a constant temperature bath then centrifuged. The amount of solute dissolved was determined by subtracting the undissolved solute, measured directly in the tube, from the total added.	SOURCE AND PURITY OF MATERIALS: (1) "Highest grade commercial sample available"; no other details given. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES:

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Durand, R. <i>C.R. Hebd. Seances Acad. Sci.</i> <u>1948</u> , 226, 409-10.
VARIABLES: One temperature: 16°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of heptane in water at 16°C was reported to be 0.015 $cm^3(1)/dm^3(2)$.</p> <p>With the assumption of a solution density of 1.00 $g\ cm^{-3}$ and a density value of 0.6868 $g\ cm^{-3}$ for heptane at 16°C (ref 2), the corresponding mass percent is 0.0010 g sln and the corresponding mole fraction, x_1, is 1.8×10^{-6} (compiler).</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>The thermostatic method described in ref 1 was used. Addition of pipetted volumes of (1) to (2) followed by shaking is repeated till appearance of turbidity.</p>	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) distilled.
ESTIMATED ERROR: soly. $\pm 0.005\ cm^3(1)/dm^3(2)$.	
REFERENCES: 1. Durand, R. <i>C.R. Hebd. Seances Acad. Sci.</i> <u>1946</u> , 223, 898-900. 2. Timmermans, J. <i>Physico-chemical constants of pure organic compounds</i> , Elsevier, 1950.	

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: McCants, J.F.; Jones, J.H.; Hopson, W.H. <i>Ind. Eng. Chem.</i> <u>1953</u> , 45, 454-6.
VARIABLES: One temperature: 100°F (311 K)	PREPARED BY: G.T. Hefter
EXPERIMENTAL VALUES: The solubility of <i>n</i> -heptane in water at 100°F (311 K) was reported to be <0.1 g(1)/100 g sln. The corresponding mole fraction, x_1 , calculated by the compiler, is $<2 \times 10^{-4}$. The solubility of water in <i>n</i> -heptane at 100°F (311 K) was reported to be 0.12 g(2)/100 g sln. The corresponding mole fraction, x_2 , calculated by the compiler, is 6.6×10^{-3} .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: The method was essentially that of ref. 1 and involved titration of the second component to the cloud point, in a constant temperature bath.	SOURCE AND PURITY OF MATERIALS: (1) Phillips; pure grade; used without further purification; n_D^{20} 1.3974. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES: 1. Washburn, E.R.; Hnizda, V.; Vold, R.D., <i>J. Am. Chem. Soc.</i> <u>1931</u> , 53, 3232.

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Guseva, A.N.; Parnov, E.I. <i>Radiokhimiya</i> <u>1963</u> , 5, 507-9.															
VARIABLES: Temperature: 71.5-187°C	PREPARED BY: A. Maczynski															
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of heptane in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>$10^5 x_1$</u></th> <th style="text-align: center;"><u>g(1)/100 g sln (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">71.5</td> <td style="text-align: center;">1.8</td> <td style="text-align: center;">0.010</td> </tr> <tr> <td style="text-align: center;">108</td> <td style="text-align: center;">2.9</td> <td style="text-align: center;">0.016</td> </tr> <tr> <td style="text-align: center;">181</td> <td style="text-align: center;">11.4</td> <td style="text-align: center;">0.0633</td> </tr> <tr> <td style="text-align: center;">187</td> <td style="text-align: center;">12.07</td> <td style="text-align: center;">0.0671</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>$10^5 x_1$</u>	<u>g(1)/100 g sln (compiler)</u>	71.5	1.8	0.010	108	2.9	0.016	181	11.4	0.0633	187	12.07	0.0671
<u>t/°C</u>	<u>$10^5 x_1$</u>	<u>g(1)/100 g sln (compiler)</u>														
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181	11.4	0.0633														
187	12.07	0.0671														
AUXILIARY INFORMATION																
METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in ref 1.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) distilled. <hr/> ESTIMATED ERROR: not specified. <hr/> REFERENCES: 1. Khazanova, P.E. <i>Tr. Gos. inst. azotn. promyshl.</i> <u>1954</u> , 4, 5.															

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Schatzberg, P. <i>J. Phys. Chem.</i> <u>1963</u> , <i>67</i> , 776-9.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of water in heptane at 25°C was reported to be 91 mg(2)/kg sln corresponding to a mole fraction, x_2 , of 5.06×10^{-4} and to a mass percent of 0.0091 g(1)/100 g sln.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: (1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20 mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.	SOURCE AND PURITY OF MATERIALS: (1) Eastman Organic Chemicals; doubly distilled; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range. (2) distilled and deionized.
	ESTIMATED ERROR: temp. \pm 0.02 K soly. 0-6% (deviations from the mean)
	REFERENCES:

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u> , 10, 42-6.																					
VARIABLES: Temperature: 0-50°C	PREPARED BY: A. Maczynski and M.C. Haulait-Pirson																					
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in heptane</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;">$t/^\circ C$</th> <th style="text-align: center;">$g(2)/100\text{ g sln}$</th> <th style="text-align: center;">$10^4 x_2$ (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0</td> <td style="text-align: center;">0.0027</td> <td style="text-align: center;">1.50</td> </tr> <tr> <td style="text-align: center;">10</td> <td style="text-align: center;">0.0054</td> <td style="text-align: center;">3.00</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.0096</td> <td style="text-align: center;">5.34</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">0.0172</td> <td style="text-align: center;">9.57</td> </tr> <tr> <td style="text-align: center;">40</td> <td style="text-align: center;">0.0308</td> <td style="text-align: center;">17.1</td> </tr> <tr> <td style="text-align: center;">50</td> <td style="text-align: center;">0.0480</td> <td style="text-align: center;">26.6</td> </tr> </tbody> </table>		$t/^\circ C$	$g(2)/100\text{ g sln}$	$10^4 x_2$ (compiler)	0	0.0027	1.50	10	0.0054	3.00	20	0.0096	5.34	30	0.0172	9.57	40	0.0308	17.1	50	0.0480	26.6
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METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostated flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. <hr/> ESTIMATED ERROR: not specified. <hr/> REFERENCES:																					

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water, H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Zel'venskii, Ya.D; Efremov, A.A.; Larin, G.M. <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u> , 10, 3-7.
VARIABLES: One temperature: 23°C	PREPARED BY: A. Maczynski
EXPERIMENTAL VALUES: <p>The solubility of water in heptane at 23°C was reported to be 0.0139 g(2)/100 g sln.</p> <p>The corresponding mole fraction, x_2, calculated by the compiler is 7.73×10^{-4}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>Saturated solutions of tritium labeled (2) in (1) were prepared in two ways. In the first, nitrogen was passed through the vessel with (2) and next through the vessel with (1) and frozen. In the second, about 500 mL of (1) and 1 mL (2) were stirred. The concentration of (2) in (1) was calculated from scintillation measurements.</p>	SOURCE AND PURITY OF MATERIALS: (1) source not specified; pure grade; shaken with conc. H ₂ SO ₄ ; washed with water, dried over sodium, and distilled; purity not specified. b.p. 98.43°C, m.p. -90.8°C. (2) source not specified; commercial; 1 Ci/mL HTO used as received.
ESTIMATED ERROR: not specified.	
REFERENCES:	

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Connolly, J.F. <i>J. Chem. Eng. Data</i> <u>1966</u> , 11, 13-6																																																																
VARIABLES: Temperature: 295-355°C Pressure: 170-700 atm	PREPARED BY: M.C. Haulait-Pirson																																																																
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of heptane in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;"><u>t/°C</u></th> <th style="text-align: left;"><u>p/atm</u></th> <th style="text-align: left;"><u>p/MPa (compiler)</u></th> <th style="text-align: left;"><u>g(l)/100 g sln</u></th> <th style="text-align: left;"><u>α₁ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td rowspan="4">295</td> <td>170</td> <td>17.22</td> <td>1.1</td> <td>0.0020</td> </tr> <tr> <td>250</td> <td>25.32</td> <td>1.1</td> <td>0.0020</td> </tr> <tr> <td>500</td> <td>50.65</td> <td>1.1</td> <td>0.0020</td> </tr> <tr> <td>700</td> <td>70.91</td> <td>1.1</td> <td>0.0020</td> </tr> <tr> <td rowspan="3">330</td> <td>200</td> <td>20.26</td> <td>3.3</td> <td>0.0061</td> </tr> <tr> <td>300</td> <td>30.39</td> <td>3.3</td> <td>0.0061</td> </tr> <tr> <td>500</td> <td>50.65</td> <td>3.3</td> <td>0.0061</td> </tr> <tr> <td rowspan="7">350</td> <td>195</td> <td>19.75</td> <td>3.7</td> <td>0.0069</td> </tr> <tr> <td>210</td> <td>21.27</td> <td>5.7</td> <td>0.0107</td> </tr> <tr> <td>260</td> <td>26.34</td> <td>9.6</td> <td>0.0187</td> </tr> <tr> <td>280</td> <td>28.36</td> <td>10.0</td> <td>0.0196</td> </tr> <tr> <td>310</td> <td>31.40</td> <td>9.6</td> <td>0.0187</td> </tr> <tr> <td>370</td> <td>37.48</td> <td>8.1</td> <td>0.0156</td> </tr> <tr> <td>550</td> <td>55.72</td> <td>5.7</td> <td>0.0107</td> </tr> </tbody> </table> <p style="text-align: right;">(continued)</p>		<u>t/°C</u>	<u>p/atm</u>	<u>p/MPa (compiler)</u>	<u>g(l)/100 g sln</u>	<u>α₁ (compiler)</u>	295	170	17.22	1.1	0.0020	250	25.32	1.1	0.0020	500	50.65	1.1	0.0020	700	70.91	1.1	0.0020	330	200	20.26	3.3	0.0061	300	30.39	3.3	0.0061	500	50.65	3.3	0.0061	350	195	19.75	3.7	0.0069	210	21.27	5.7	0.0107	260	26.34	9.6	0.0187	280	28.36	10.0	0.0196	310	31.40	9.6	0.0187	370	37.48	8.1	0.0156	550	55.72	5.7	0.0107
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METHOD/APPARATUS/PROCEDURE: The cloud point method was used. Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected, until either a cloud or a small portion of a second phase appeared at the top of the cell. Then mercury was injected to change the pressure, more (1) was injected and the procedure was repeated.	SOURCE AND PURITY OF MATERIALS: (1) Phillips reagent grade; better than 99.8%; used as received. (2) distilled and deaerated. ESTIMATED ERROR: temp. ± 0.02 K press. ± 2 atm (accuracy) REFERENCES:																																																																

COMPONENTS:

- (1) Heptane; C_7H_{16} ; [142-82-5]
 (2) Water; H_2O ; [7732-18-5]

ORIGINAL MEASUREMENTS:

Connolly, J.F.
J. Chem. Eng. Data 1966, 11, 13-6.

$t/^\circ C$	p/atm	p/MPa (compiler)	$g(1)/100\ g\ sln$	x_1 (compiler)
355	230	23.30	10.3	0.0202
	240	24.31	13.5	0.0273
	250	25.32	19.5	0.0417
	245	24.82	24.7	0.0557
	320	32.42	41.7	0.1139
	310	31.40	35.7	0.0885
	300	30.39	29.3	0.0693
	300	30.39	24.8	0.0559
	305	30.90	19.5	0.0417
	345	34.95	13.5	0.0273
	390	39.51	10.3	0.0202

COMMENTS AND ADDITIONAL DATA:

Upper critical solution temperature: $353^\circ C$ at $p = 290\ atm$ (29.83 MPa).

The uncertainty in the CST is about $2^\circ C$ and that of the corresponding pressure about 10 atm.

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u> , 70, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of heptane in water at 25°C was reported to be 2.93 mg (1)/kg sln (0.000293 g(1)/100 g sln). The corresponding mole fraction, x_1 , calculated by the compiler, is 5.3×10^{-7} . The same value is also reported in refs 1 and 2.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μ L sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5 K soly. 0.20 mg (1)/kg sln (standard deviation from mean) REFERENCES: 1. McAuliffe, C. <i>Nature (London)</i> <u>1963</u> , 200, 1092. 2. McAuliffe, C. <i>Am. Chem. Soc. Div. Petrol. Chem.</i> <u>1964</u> , 9, 275.

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Nelson, H.D.; De Ligny, C.L. <i>Rec. Trav. Chim. Pays-Bas</i> <u>1968</u> , 87, 528-44.																		
VARIABLES: Temperature: 4.3-45°C	PREPARED BY: M.C. Haulait-Pirson																		
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of heptane in water</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;">$t/^\circ C$</th> <th style="text-align: center;">$10^7 x_1$</th> <th style="text-align: center;">mg(1)/kg sln (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">4.3</td> <td style="text-align: center;">3.51 ± 0.26</td> <td style="text-align: center;">1.95</td> </tr> <tr> <td style="text-align: center;">13.5</td> <td style="text-align: center;">3.63 ± 0.51</td> <td style="text-align: center;">2.02</td> </tr> <tr> <td style="text-align: center;">25.0</td> <td style="text-align: center;">4.78 ± 0.74</td> <td style="text-align: center;">2.66</td> </tr> <tr> <td style="text-align: center;">35.0</td> <td style="text-align: center;">4.07 ± 0.95</td> <td style="text-align: center;">2.27</td> </tr> <tr> <td style="text-align: center;">45.0</td> <td style="text-align: center;">4.32 ± 1.06</td> <td style="text-align: center;">2.41</td> </tr> </tbody> </table>		$t/^\circ C$	$10^7 x_1$	mg(1)/kg sln (compiler)	4.3	3.51 ± 0.26	1.95	13.5	3.63 ± 0.51	2.02	25.0	4.78 ± 0.74	2.66	35.0	4.07 ± 0.95	2.27	45.0	4.32 ± 1.06	2.41
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METHOD/APPARATUS/PROCEDURE: The saturation vessel is drawn in the original paper. (2) was saturated with (1) via the vapor phase: a few drops of (1) were put on the bottom of a tight-fitting flask containing a small flask filled with water. Complete saturation was reached by shaking overnight in an upright position. Samples were taken from the aqueous solution with a microsyringe through the septum and injected into the gas chromatograph equipped with a flame ionization detector. The gas chromatographic conditions are described in the paper.	SOURCE AND PURITY OF MATERIALS: (1) Phillips pure grade. (2) tap-water was refluxed for 8 hours in the presence of $KMnO_4$ and KOH and distilled. The whole process was repeated once more. ESTIMATED ERROR: soly.: error given above (90% probability interval)																		
	REFERENCES:																		

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Ghanem, N.A.; Marek, M.; Exner, J. <i>Int. J. Appl. Radiat. Isotop.</i> <u>1970</u> , 21, 239-40.
VARIABLES: One temperature: 22.5°	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of water in heptane at 22.5°C was reported to be 3.93×10^{-3} g(2)/100 mL (1) or 5.73×10^{-3} g(2)/100 g (1). The corresponding mass percent and mole fraction, x_2 , calculated by the compiler are 5.73×10^{-3} g(2)/100 g sln and 3.19×10^{-4} .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: A volume of standardized radioactive water was injected in a vessel containing dry (1). The vessel was then closed and the contents were shaken and stirred. The vessel was then left for the excess water to settle to the bottom and sides and to ensure equilibrium. Portions of (1) saturated with (2) were added to a scintillation mixture and counted.	SOURCE AND PURITY OF MATERIALS: (1) source not specified; purified by shaking with a mixture of H ₂ SO ₄ and P ₂ O ₅ , kept over KOH, then distilled and the distillate refluxed over NaH; residual water content $< 5 \times 10^{-6}$ mol·dm ⁻³ (2) not specified. ESTIMATED ERROR: temp. ± 1 K soly. ± 10% (type of error not specified) REFERENCES:

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. <i>Neftekhimiya</i> <u>1973</u> , 13, 885-7.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski
EXPERIMENTAL VALUES: <p>The solubility of heptane in water at 25°C was reported to be $x_1 = 5.0 \times 10^{-7}$.</p> <p>The corresponding mass percent calculated by the compiler is 2.8×10^{-4} g(1)/100 g sln.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigorously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.</p>	SOURCE AND PURITY OF MATERIALS: (1) source not specified; CP reagent; purity not specified. (2) distilled. ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Polak, J.; Lu, B.C-Y. <i>Can. J. Chem.</i> <u>1973</u> , <i>51</i> , 4018-23.																		
VARIABLES: Temperature: 0-25°C	PREPARED BY: M.C. Haulait-Pirson																		
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of heptane in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>mg(1)/kg sln</u></th> <th style="text-align: center;"><u>x₁ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0^a</td> <td style="text-align: center;">4.39^c</td> <td style="text-align: center;">7.9 x 10⁻⁷</td> </tr> <tr> <td style="text-align: center;">25^b</td> <td style="text-align: center;">3.37^c</td> <td style="text-align: center;">6.1 x 10⁻⁷</td> </tr> </tbody> </table> <p style="text-align: center;">Solubility of water in heptane</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>mg(2)/kg sln</u></th> <th style="text-align: center;"><u>x₂ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0^a</td> <td style="text-align: center;">26^d</td> <td style="text-align: center;">1.45 x 10⁻⁴</td> </tr> <tr> <td style="text-align: center;">25^b</td> <td style="text-align: center;">82^e</td> <td style="text-align: center;">4.56 x 10⁻⁴</td> </tr> </tbody> </table> <p>a-e see "ESTIMATED ERROR"</p>		<u>t/°C</u>	<u>mg(1)/kg sln</u>	<u>x₁ (compiler)</u>	0 ^a	4.39 ^c	7.9 x 10 ⁻⁷	25 ^b	3.37 ^c	6.1 x 10 ⁻⁷	<u>t/°C</u>	<u>mg(2)/kg sln</u>	<u>x₂ (compiler)</u>	0 ^a	26 ^d	1.45 x 10 ⁻⁴	25 ^b	82 ^e	4.56 x 10 ⁻⁴
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AUXILIARY INFORMATION																			
METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.																		
ESTIMATED ERROR: temp. a) ± 0.02 K; b) ± 0.01 K soly. c) ± 4%; d) ± 4.7%; e) ± 3.1% (mean)																			
REFERENCES:																			

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S. <i>Zh. Fiz. Khim.</i> 1976, 50, 1344. Deposited doc. 1976, VINITI 437-76.																		
VARIABLES: Temperature: 20 and 40°C	PREPARED BY: A. Maczynski																		
EXPERIMENTAL VALUES: <div style="text-align: center;">Solubility of heptane in water</div> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th>$t/^\circ C$</th> <th>$10^5 x_1$</th> <th>$10^3 \text{ g(1)/100 g sln (compiler)}$</th> </tr> </thead> <tbody> <tr> <td>20</td> <td>0.3</td> <td>2</td> </tr> <tr> <td>40</td> <td>1</td> <td>6</td> </tr> </tbody> </table> <div style="text-align: center;">Solubility of water in heptane</div> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th>$t/^\circ C$</th> <th>$10^4 x_2$</th> <th>$10^3 \text{ g(2)/100 g sln (compiler)}$</th> </tr> </thead> <tbody> <tr> <td>20</td> <td>5</td> <td>9</td> </tr> <tr> <td>40</td> <td>7</td> <td>13</td> </tr> </tbody> </table>		$t/^\circ C$	$10^5 x_1$	$10^3 \text{ g(1)/100 g sln (compiler)}$	20	0.3	2	40	1	6	$t/^\circ C$	$10^4 x_2$	$10^3 \text{ g(2)/100 g sln (compiler)}$	20	5	9	40	7	13
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METHOD/APPARATUS/PROCEDURE: Nothing specified in the paper.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: Not specified. REFERENCES:																		

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Price, L.C. <i>Am. Assoc. Petrol. Geol. Bull.</i> <u>1976, 60, 213-44.</u>																																
VARIABLES: Temperature: 25-150.4°C	PREPARED BY: F. Kapuku																																
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of heptane in water at system pressure</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>mg(1)/kg(2)</u></th> <th style="text-align: center;"><u>g(1)/100 g sln (compiler)</u></th> <th style="text-align: center;"><u>$10^7 x_1$ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">25.0</td> <td style="text-align: center;">2.24 ± 0.04</td> <td style="text-align: center;">0.000224</td> <td style="text-align: center;">4.0</td> </tr> <tr> <td style="text-align: center;">40.1</td> <td style="text-align: center;">2.63 ± 0.05</td> <td style="text-align: center;">0.000263</td> <td style="text-align: center;">4.7</td> </tr> <tr> <td style="text-align: center;">55.7</td> <td style="text-align: center;">3.11 ± 0.11</td> <td style="text-align: center;">0.000311</td> <td style="text-align: center;">5.6</td> </tr> <tr> <td style="text-align: center;">99.1</td> <td style="text-align: center;">5.60 ± 0.17</td> <td style="text-align: center;">0.000560</td> <td style="text-align: center;">10.1</td> </tr> <tr> <td style="text-align: center;">118.0</td> <td style="text-align: center;">11.4 ± 0.4</td> <td style="text-align: center;">0.00114</td> <td style="text-align: center;">20.5</td> </tr> <tr> <td style="text-align: center;">136.6</td> <td style="text-align: center;">27.3 ± 0.9</td> <td style="text-align: center;">0.00273</td> <td style="text-align: center;">49.1</td> </tr> <tr> <td style="text-align: center;">150.4</td> <td style="text-align: center;">43.7 ± 1.0</td> <td style="text-align: center;">0.00437</td> <td style="text-align: center;">78.6</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>mg(1)/kg(2)</u>	<u>g(1)/100 g sln (compiler)</u>	<u>$10^7 x_1$ (compiler)</u>	25.0	2.24 ± 0.04	0.000224	4.0	40.1	2.63 ± 0.05	0.000263	4.7	55.7	3.11 ± 0.11	0.000311	5.6	99.1	5.60 ± 0.17	0.000560	10.1	118.0	11.4 ± 0.4	0.00114	20.5	136.6	27.3 ± 0.9	0.00273	49.1	150.4	43.7 ± 1.0	0.00437	78.6
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AUXILIARY INFORMATION																																	
METHOD/APPARATUS/PROCEDURE: <p>Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and insured saturation (in 2 to 4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.</p>	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1 K soly. range of values given above REFERENCES:																																

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977.04.05 C.A. 87:87654.
VARIABLES: One temperature: 20°C	PREPARED BY: A. Maczynski
EXPERIMENTAL VALUES: <p>The solubility of heptane in water at 20°C was reported to be 0.06 g(l)dm⁻³(2).</p> <p>The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.006 g(l)/100 g sln and 1.1×10^{-5}. The assumption that 1 dm³ sln = 1 kg sln was used in the calculation.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>About 100-500 mL(2) was placed in a glass cylinder and 10-50 mg of an insoluble indicator was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall 2-3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5-1.5 min.</p>	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS: (1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Bittrich, H.-J.; Gedan, H.; Feix, G. <i>Z. Phys. Chem., Leipzig</i> <u>1979</u> , 260, 1009-13.																				
VARIABLES: Temperature: 25-40°C	PREPARED BY: M.C. Haulait-Pirson																				
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of heptane in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;"><u>t/°C</u></th> <th style="text-align: center;"><u>mg(1)/kg(2)</u></th> <th style="text-align: center;"><u>g(1)/100 g sln (compiler)</u></th> <th style="text-align: center;"><u>x₁ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td>unspecified</td> <td style="text-align: center;">3.7</td> <td style="text-align: center;">0.00037</td> <td style="text-align: center;">6.6 x 10⁻⁷</td> </tr> </tbody> </table> <p style="text-align: center;">Solubility of water in heptane</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;"><u>t/°C</u></th> <th style="text-align: center;"><u>mg(2)/kg(1)</u></th> <th style="text-align: center;"><u>g(2)/100 g sln (compiler)</u></th> <th style="text-align: center;"><u>x₂ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td>25</td> <td style="text-align: center;">121</td> <td style="text-align: center;">0.0121</td> <td style="text-align: center;">6.73 x 10⁻⁴</td> </tr> <tr> <td>40</td> <td style="text-align: center;">156</td> <td style="text-align: center;">0.0156</td> <td style="text-align: center;">8.68 x 10⁻⁴</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>mg(1)/kg(2)</u>	<u>g(1)/100 g sln (compiler)</u>	<u>x₁ (compiler)</u>	unspecified	3.7	0.00037	6.6 x 10 ⁻⁷	<u>t/°C</u>	<u>mg(2)/kg(1)</u>	<u>g(2)/100 g sln (compiler)</u>	<u>x₂ (compiler)</u>	25	121	0.0121	6.73 x 10 ⁻⁴	40	156	0.0156	8.68 x 10 ⁻⁴
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METHOD/APPARATUS/PROCEDURE: A mixture of (1) and (2) was shaken with no access of air at a specified temperature and then thermostatted for 48 hr. The equilibrated phases were sampled and analysed by gas chromatography using a flame-ionization detector. A 3-m-steel column of 15% nitril silicone on Porolith, 110°C and a 3-m-steel column of 1.5 g CaC ₂ and 10% SE 30 on chromaton N, 120°C were used for (1) and (2) respectively.	SOURCE AND PURITY OF MATERIALS: (1) source not specified; distilled or crystallized; purity tested by gas chromatography. (2) not specified. ESTIMATED ERROR: soly. ± 9% (type of error not specified). REFERENCES:																				

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Rudakov, E.S.; Lutsyk, A.I. <i>Zh. Fiz. Khim.</i> <u>1979</u> , <i>53</i> , 1298-1300.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The authors reported the partition coefficient α of heptane between the gas and aqueous phase. $\alpha = 84 \pm 4$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25°C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).</p> <p>The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of p (where p is the vapor pressure in mm of Hg) is taken from ref 1. $p = 45.81$ mm of Hg and $\log C_g = \log p - 4.269 = -2.61$ expressed in moles per liter. Therefore $C_s = 2.9 \times 10^{-5}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is $0.00029 \text{ g(1)/100 g soln}$ and the corresponding mole fraction, x_1, is 5.2×10^{-7}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.</p>	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: soly. $\pm 10\%$ (estimated by the compiler) REFERENCES: 1. Hine, J.; Mooker, P.K. <i>J. Org. Chem.</i> <u>1975</u> , <i>4</i> , 292.

<p>COMPONENTS:</p> <p>(1) Heptane; C_7H_{16}; [142-82-5]</p> <p>(2) Water; H_2O; [7732-18-5]</p>	<p>ORIGINAL MEASUREMENTS:</p> <p>Jonsson, J.A.; Vejrosta, J.; Novak, J.</p> <p><i>Fluid Phase Equil.</i> <u>1982</u>, 9, 279-86.</p>																												
<p>VARIABLES:</p> <p>Temperature: 15-35°C</p>	<p>PREPARED BY:</p> <p>G.T. Hefter</p>																												
<p>EXPERIMENTAL VALUES:</p> <table border="1" data-bbox="266 510 1220 768"> <thead> <tr> <th colspan="4" style="text-align: center;">Solubility of heptane in water</th> </tr> <tr> <th style="text-align: center;">$t/^\circ C$</th> <th style="text-align: center;">mg(1)/kg sln</th> <th style="text-align: center;">$10^4 g(1)/100g\ sln$ (compiler)</th> <th style="text-align: center;">$10^7 x_1$ (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">15</td> <td style="text-align: center;">2.67</td> <td style="text-align: center;">2.67</td> <td style="text-align: center;">4.80</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">2.57</td> <td style="text-align: center;">2.57</td> <td style="text-align: center;">4.62</td> </tr> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">2.51</td> <td style="text-align: center;">2.51</td> <td style="text-align: center;">4.51</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">2.49</td> <td style="text-align: center;">2.49</td> <td style="text-align: center;">4.47</td> </tr> <tr> <td style="text-align: center;">35</td> <td style="text-align: center;">2.52</td> <td style="text-align: center;">2.52</td> <td style="text-align: center;">4.53</td> </tr> </tbody> </table> <p>^a Solubility values were calculated by the authors from their smoothed air-water partition coefficient (K_{AW}) by assuming K_{AW} values obtained at infinite dilution were valid at the saturation pressure of (1).</p>		Solubility of heptane in water				$t/^\circ C$	mg(1)/kg sln	$10^4 g(1)/100g\ sln$ (compiler)	$10^7 x_1$ (compiler)	15	2.67	2.67	4.80	20	2.57	2.57	4.62	25	2.51	2.51	4.51	30	2.49	2.49	4.47	35	2.52	2.52	4.53
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<p>METHOD/APPARATUS/PROCEDURE:</p> <p>Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapour concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and the entrapped (1) analysed by gas chromatography. The method and apparatus are described in detail in ref 1.</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p>(1) Fluka, > 99.7%, used as received.</p> <p>(2) Not specified.</p> <p>ESTIMATED ERROR:</p> <p>Not specified.</p> <p>REFERENCES:</p> <p>1. Vejrosta, J.; Novak, J.; Jonsson, J.A. <i>Fluid Phase Equil.</i> <u>1982</u>, 8, 25-35.</p>																												

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Deuterium oxide (heavy water); D_2O ; [7789-20-0]	ORIGINAL MEASUREMENTS: Guseva, A.N.; Parnov, E.I. <i>Radiokhimiya</i> <u>1963</u> , 5, 507-9.															
VARIABLES: Temperature: 68-193°C	PREPARED BY: A. Maczynski															
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of heptane in deuterium oxide</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;">$t/^\circ C$</th> <th style="text-align: center;">$10^5 x_1$</th> <th style="text-align: center;">$g(l)/100 g \text{ sln (compiler)}$</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">68</td> <td style="text-align: center;">1.51</td> <td style="text-align: center;">0.0076</td> </tr> <tr> <td style="text-align: center;">109</td> <td style="text-align: center;">2.8</td> <td style="text-align: center;">0.0140</td> </tr> <tr> <td style="text-align: center;">158</td> <td style="text-align: center;">6.24</td> <td style="text-align: center;">0.0312</td> </tr> <tr> <td style="text-align: center;">193</td> <td style="text-align: center;">14.9</td> <td style="text-align: center;">0.0745</td> </tr> </tbody> </table>		$t/^\circ C$	$10^5 x_1$	$g(l)/100 g \text{ sln (compiler)}$	68	1.51	0.0076	109	2.8	0.0140	158	6.24	0.0312	193	14.9	0.0745
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METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in ref 1.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) distilled. ESTIMATED ERROR: not specified. REFERENCES: 1. Khazanova, P.E. <i>Tr. Gos. inst. azotn. promyshl.</i> <u>1954</u> , 4, 5.															

COMPONENTS:		EVALUATOR:		
(1) Heptane; C ₇ H ₁₆ ; [142-82-5] (2) Seawater		D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982		
CRITICAL EVALUATION:				
The solubility of heptane (1) in seawater (2) has been reported in two works:				
Authors	Method	T/K	Salinity g salts/kg sln	g(1)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	298	6	1.03 x 10 ⁻³
Freegarde <i>et al.</i> (ref 2)	GLC	?	?	4 x 10 ⁻⁴
Because temperature and salinity are not specified, the data of Freegarde <i>et al.</i> are rejected. The value of Krasnoshchekova and Gubergrits is considered doubtful since it is greater than the tentative value for the solubility of heptane in pure water at 298 K.				
<u>SOLUBILITY OF HEPTANE (1) IN SEAWATER (2)</u>				
<u>DOUBTFUL VALUE</u>				
T/K	g salts/kg sln		g(1)/100 g sln	
298	6		1.03 x 10 ⁻³	
REFERENCES				
1. Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. <i>Neftekhimiya</i> <u>1973</u> , <i>13</i> , 885-8.				
2. Freegarde, M., Hatchard, C.G.; Parker, C.A. <i>Lab. Pract.</i> <u>1971</u> , <i>20</i> , 35-40.				

COMPONENTS: (1) Heptane; C_7H_{16} ; [142-82-5] (2) Seawater	ORIGINAL MEASUREMENTS: Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. <i>Neftekhimiya</i> <u>1973</u> , 13, 885-8.
VARIABLES: One temperature: 25°C Salinity: 6 g/kg sln	PREPARED BY: M. Kleinschmidt
EXPERIMENTAL VALUES: <p>The solubility of heptane in seawater was reported to be 1.03×10^{-3} g(l)/100 g sln. and the corresponding mole fraction, $x_1 = 1.9 \times 10^{-6}$.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.</p>	SOURCE AND PURITY OF MATERIALS: (1) "chemically pure" (2) distilled water plus salt mixture. <hr/> ESTIMATED ERROR: not specified. <hr/> REFERENCES:

