

<p>COMPONENTS:</p> <p>(1) Octane; C₈H₁₈; [111-65-9]</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>
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CRITICAL EVALUATION:

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

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

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

^a High pressure data

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

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

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

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

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

(continued next page)

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

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

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

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

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

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

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

(Table 2 continued next page)

COMPONENTS:

- (1) Octane; C_8H_{18} ; [111-65-9]
 (2) Water; H_2O ; [7732-18-5]

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CRITICAL EVALUATION: (continued)

TABLE 2 (continued)

T/K	Solubility values		
	Reported values $10^4 g(1)/100g \text{ sln}$	"Best" values ($\pm \sigma_n$) ^a $10^4 g(1)/100g \text{ sln}$	$10^7 x_1$
393	4.5 ^b (ref 12), 7.23 ^c (ref 16)	7.2	11
413	9.5 ^b (ref 12), 15.1 ^c (ref 16)	15	24
433	12.0 ^b (ref 12), 22.2 ^c (ref 16)	22	35

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Data from ref 12 have been excluded in the calculation of "Best" values, see text.

^b Obtained by the Evaluator by graphical interpolation of the author's original data.

^c Calculated from the authors' fitting equation over the range of their experimental values.

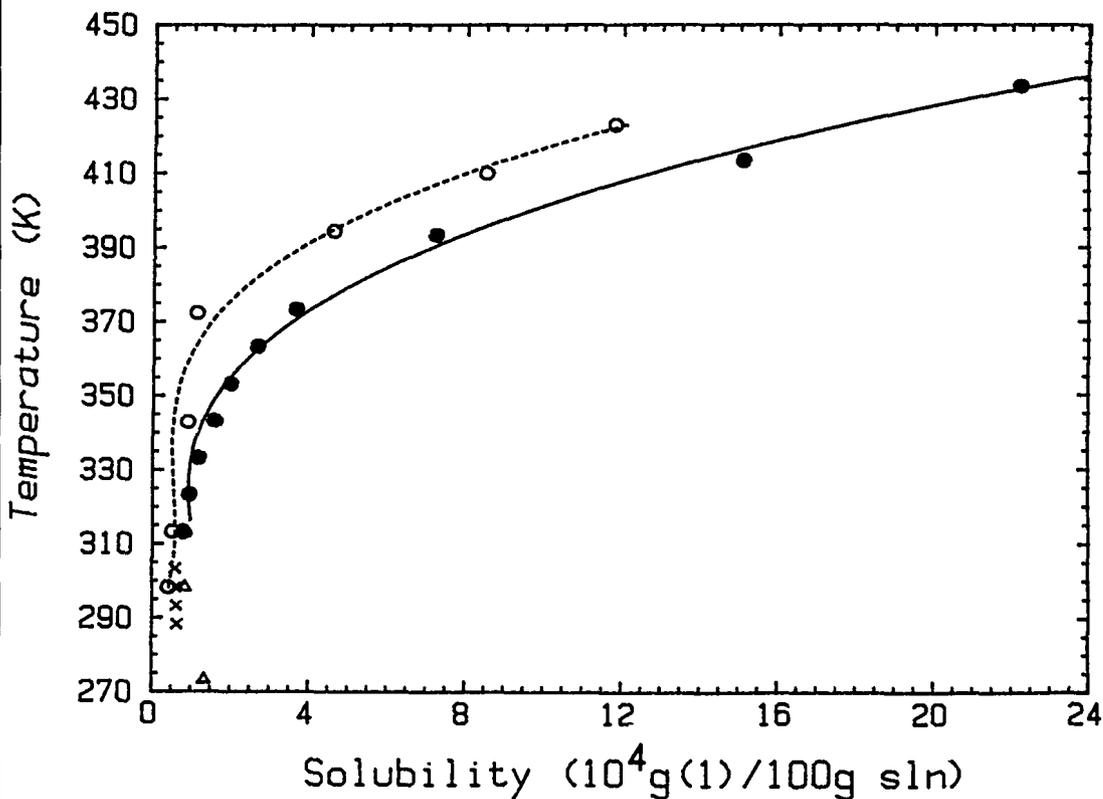


FIGURE 1. Solubility of octane in water, selected data: ref 10 (Δ); ref 12 (o); ref 15 (x); ref 16 (\bullet).

(continued next page)

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

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

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

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

T/K	Solubility values		
	Reported values 10 ² g(2)/100g sln	"Best" values (± σ _n) ^a 10 ² g(2)/100g sln	10 ⁴ x ₂
273	0.23 (ref 9)	0.2	1
283	0.51 (ref 4)	0.5	3
293	0.95 (ref 4), 0.68 (ref 10)	0.8 ± 0.1	5
298	1.26 ^b (ref 4), 0.79 (ref 9)	1.0 ± 0.2	6
303	1.68 (ref 4)	1.7	11
313	1.58 ^c (ref 14)	1.6	10
323	2.40 ^c (ref 14)	2.4	15
333	3.54 ^c (ref 14)	3.5	22
343	5.14 ^c (ref 14)	5.1	32
353	7.30 ^c (ref 14)	7.3	46
363	10.2 ^c (ref 14)	10	63
373	14.0 ^c (ref 14)	14	89

a Obtained by averaging where appropriate; σ_n has no statistical significance.

b Obtained by graphical interpolation (Evaluator) of authors' original data.

c Calculated (Evaluator) from fitting equation given by authors, over the range of their experimental values.

(continued next page)

COMPONENTS:

- (1) Octane; C_8H_{18} ; [111-65-9]
 (2) Water; H_2O ; [7732-18-5]

EVALUATOR:

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 and Physical Sciences, Murdoch
 University, Perth, W.A., Australia.
 October 1986.

CRITICAL EVALUATION: (continued)

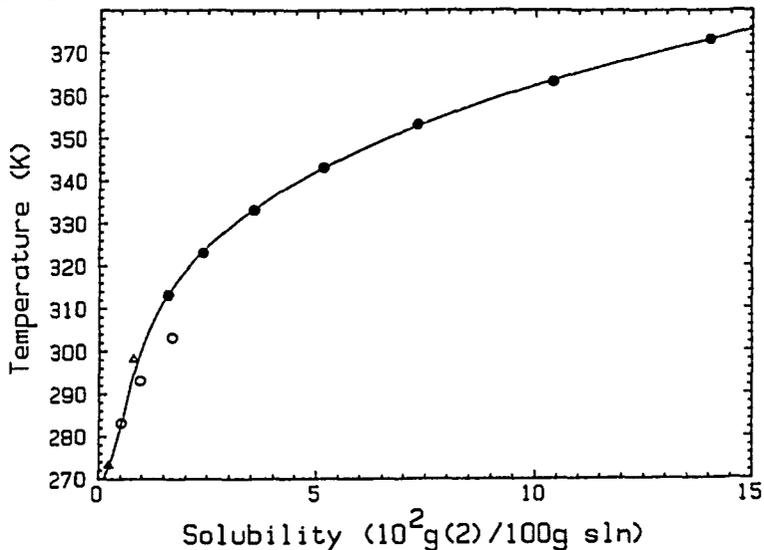


FIGURE 2. Solubility of water in octane; ref 4 (○); ref 10 (△); ref 16 (●). Solid line has been fitted to "Best" values in Table 3.

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

This system exhibits phase behaviour which is topographically similar to that of benzene + water, *i.e.*, it belongs to type III phase behaviour using Scott and von Konynenburg's (ref 17) classification (see Figure 3 and the Introduction to this volume).

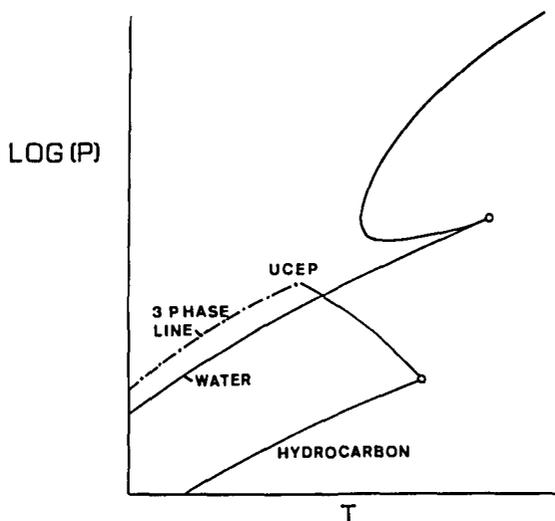


FIGURE 3. Pressure-temperature projection of the equilibrium pressure-temperature composition surface for type III phase behaviour. (continued next page)

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

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

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

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

a Critical point of unspecified composition.

b Along the three-phase line.

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

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

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

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1. Fühner, H. *Chem. Ber.* 1924, *57*, 510-5.
2. Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* 1948, *16*, 537-48.
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4. Englin, B.A., Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. *Tekhnol. Topl. Masel* 1965, *10*, 42-6.
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13. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.
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16. Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. *A.I.Ch.E.J.* 1985, *31*, 376-84.
17. Scott, R.L.; van Konynenburg, P.H. *Phil. Trans. Roy. Soc. London* 1980, *A298*, 495.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

*NOTE ADDED IN PROOF

Delete ref 7.

COMPONENTS: (1) Octane; C_8H_{18} ; [111-65-9] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Fühner, H. <i>Ber. Dtsh. Chem. Ges.</i> <u>1924</u> , 57, 510-5.
VARIABLES: One temperature: 16°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of octane in water at 16°C was reported to be 0.002 mL(1)/100 mL sln or 0.0014 g(1)/100 g sln. The corresponding mole fraction, x_1 , calculated by the compiler is 0.22×10^{-5} .	
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) Octane; C_8H_{18} ; [111-65-9] (2) Water; H_2O ; [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: One temperature: 20°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of water in octane at 20°C and at a total saturation pressure of 1 atm was reported to be 0.0142 g(2)/100 g(1). The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 0.0142 g(2)/100 g sln and 9.0×10^{-4}.</p>	
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) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Baker, E.G. <i>Geochim. Cosmochim. Acta</i> <u>1960</u> , 19, 309-17.
VARIABLES: One temperature: not specified.	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of octane in water was reported to be 0.09×10^{-6} mL (1)/mL (2).	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined after ultrafiltration using the procedure described in ref 1.	SOURCE AND PURITY OF MATERIALS: not specified. ESTIMATED ERROR: not specified. REFERENCES: 1. Baker, E.G. <i>Am. Chem. Soc., Div. Petrol. Chem., Preprint</i> <u>1958</u> , 3, N°4, C61.

COMPONENTS: (1) Octane; C_8H_{18} ; [111-65-9] (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. Masei</i> <u>1965</u> , 10, 42-6.												
VARIABLES: Temperature: 10-30°C	PREPARED BY: A. Maczynski and M.C. Haulait-Pirson												
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in octane</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <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;">10</td> <td style="text-align: center;">0.0051</td> <td style="text-align: center;">3.24</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.0095</td> <td style="text-align: center;">6.03</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">0.0168</td> <td style="text-align: center;">10.65</td> </tr> </tbody> </table>		$t/^\circ C$	$g(2)/100\text{ g sln}$	$10^4 x_2$ (compiler)	10	0.0051	3.24	20	0.0095	6.03	30	0.0168	10.65
$t/^\circ C$	$g(2)/100\text{ g sln}$	$10^4 x_2$ (compiler)											
10	0.0051	3.24											
20	0.0095	6.03											
30	0.0168	10.65											
AUXILIARY INFORMATION													
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: not specified. REFERENCES:												

COMPONENTS: (1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u> , <i>70</i> , 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of octane in water at 25°C was reported to be 0.66 mg (1)/kg sln.</p> <p>The corresponding mole fraction, x_1, calculated by the compiler, is 1.04×10^{-7}.</p> <p>The same value is also reported in refs 1 and 2.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>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 μL 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.</p>	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled. ESTIMATED ERROR: temp. $\pm 1.5^\circ\text{C}$ soly. 0.06 mg (1)/kg sln (standard deviation from mean) REFERENCES: 1. McAuliffe, C. <i>Nature (London)</i> <u>1963</u> , <i>200</i> , 1092. 2. McAuliffe, C. <i>Am. Chem. Soc., Div. Petrol. Chem.</i> <u>1964</u> , <i>9</i> , 275.

COMPONENTS: (1) Octane; C_8H_{18} ; [111-65-9] (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: 5-45°C	PREPARED BY: M.C. Haulait-Pirson												
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of octane 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(l)/kg sln (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">5.0</td> <td style="text-align: center;">2.6 ± 0.6</td> <td style="text-align: center;">1.65</td> </tr> <tr> <td style="text-align: center;">15.0</td> <td style="text-align: center;">1.4 ± 0.6</td> <td style="text-align: center;">0.89</td> </tr> <tr> <td style="text-align: center;">45.0</td> <td style="text-align: center;">2.9 ± 0.6</td> <td style="text-align: center;">1.84</td> </tr> </tbody> </table>		$t/^\circ C$	$10^7 x_1$	mg(l)/kg sln (compiler)	5.0	2.6 ± 0.6	1.65	15.0	1.4 ± 0.6	0.89	45.0	2.9 ± 0.6	1.84
$t/^\circ C$	$10^7 x_1$	mg(l)/kg sln (compiler)											
5.0	2.6 ± 0.6	1.65											
15.0	1.4 ± 0.6	0.89											
45.0	2.9 ± 0.6	1.84											
AUXILIARY INFORMATION													
METHOD/APPARATUS/PROCEDURE: <p>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.</p>	SOURCE AND PURITY OF MATERIALS: (1) Fluka purum. (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 (standard deviation) REFERENCES:												

COMPONENTS: (1) Octane; C ₈ H ₁₈ ; [111-65-9] (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 octane in water at 25°C was reported to be $x_1 = 1.0 \times 10^{-7}$. The corresponding mass percent calculated by the compiler is 7.0×10^{-5} 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) Octane; C_8H_{18} ; [111-65-9] (2) Water; H_2O ; [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 octane in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <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;">x_1 (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0^a</td> <td style="text-align: center;">1.35^c</td> <td style="text-align: center;">2.13×10^{-7}</td> </tr> <tr> <td style="text-align: center;">25^b</td> <td style="text-align: center;">0.85^c</td> <td style="text-align: center;">1.34×10^{-7}</td> </tr> </tbody> </table> <p style="text-align: center;">Solubility of water in octane</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;">$t/^\circ C$</th> <th style="text-align: center;">mg(2)/kg sln</th> <th style="text-align: center;">x_2 (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0^a</td> <td style="text-align: center;">23^d</td> <td style="text-align: center;">1.46×10^{-4}</td> </tr> <tr> <td style="text-align: center;">25^b</td> <td style="text-align: center;">79^e</td> <td style="text-align: center;">5.01×10^{-4}</td> </tr> </tbody> </table> a-e See "Estimated Error"		$t/^\circ C$	mg(1)/kg sln	x_1 (compiler)	0 ^a	1.35 ^c	2.13×10^{-7}	25 ^b	0.85 ^c	1.34×10^{-7}	$t/^\circ C$	mg(2)/kg sln	x_2 (compiler)	0 ^a	23 ^d	1.46×10^{-4}	25 ^b	79 ^e	5.01×10^{-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) $\pm 0.02^\circ C$; b) $\pm 0.01^\circ C$ soly. c) $\pm 4\%$; d) $\pm 4.7\%$; e) $\pm 3.1\%$ (mean)																			
REFERENCES:																			

COMPONENTS: (1) Octane; C_8H_{18} ; [111-65-9] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S. <i>Zh. Fiz. Khim.</i> <u>1976</u> , 50, 1344. <i>Deposited doc.</i> <u>1976</u> , VINITI 437-76.
VARIABLES: One temperature: 20°C	PREPARED BY: A. Maczynski
EXPERIMENTAL VALUES: The solubility of octane in water at 20°C was reported to be $x_1 \approx 2 \times 10^{-7}$. The corresponding mass percent calculated by the compiler is about 0.0001 g(1)/100 g sln. The solubility of water in octane at 20°C was reported to be $x_2 = 4.3 \times 10^{-4}$. The corresponding mass percent calculated by the compiler is 0.007 g(2)/100 g sln.	
AUXILIARY INFORMATION	
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) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Price, L.C. <i>Am. Assoc. Petrol. Geol. Bull.</i> <u>1976, 60, 213-44.</u>																																
VARIABLES: Temperature: 25-149.5°C	PREPARED BY: F. Kapuku																																
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of octane 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>10⁷x₁ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">25.0</td> <td style="text-align: center;">0.431 ± 0.012</td> <td style="text-align: center;">0.0000431</td> <td style="text-align: center;">0.680</td> </tr> <tr> <td style="text-align: center;">40.1</td> <td style="text-align: center;">0.524 ± 0.021</td> <td style="text-align: center;">0.0000524</td> <td style="text-align: center;">0.826</td> </tr> <tr> <td style="text-align: center;">69.7</td> <td style="text-align: center;">0.907 ± 0.042</td> <td style="text-align: center;">0.0000907</td> <td style="text-align: center;">1.43</td> </tr> <tr> <td style="text-align: center;">99.1</td> <td style="text-align: center;">1.12 ± 0.07</td> <td style="text-align: center;">0.000112</td> <td style="text-align: center;">1.77</td> </tr> <tr> <td style="text-align: center;">121.3</td> <td style="text-align: center;">4.62 ± 0.22</td> <td style="text-align: center;">0.000462</td> <td style="text-align: center;">7.29</td> </tr> <tr> <td style="text-align: center;">136.6</td> <td style="text-align: center;">8.52 ± 0.34</td> <td style="text-align: center;">0.000852</td> <td style="text-align: center;">13.4</td> </tr> <tr> <td style="text-align: center;">149.5</td> <td style="text-align: center;">11.80 ± 0.7</td> <td style="text-align: center;">0.00118</td> <td style="text-align: center;">18.6</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>mg(1)/kg(2)</u>	<u>g(1)/100 g sln (compiler)</u>	<u>10⁷x₁ (compiler)</u>	25.0	0.431 ± 0.012	0.0000431	0.680	40.1	0.524 ± 0.021	0.0000524	0.826	69.7	0.907 ± 0.042	0.0000907	1.43	99.1	1.12 ± 0.07	0.000112	1.77	121.3	4.62 ± 0.22	0.000462	7.29	136.6	8.52 ± 0.34	0.000852	13.4	149.5	11.80 ± 0.7	0.00118	18.6
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AUXILIARY INFORMATION																																	
METHOD/APPARATUS/PROCEDURE: 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.	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. range of values given above REFERENCES:																																

COMPONENTS: (1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water, H ₂ O; [7732-18-5]		ORIGINAL MEASUREMENTS: Skripka, V.G. <i>Tr. Vses. Neftegazov. Nauch. Issled. Inst.</i> <u>1976</u> , 61, 139-51. Sultanov, R.G.; Skripka, V.G. <i>Zh. Fiz. Khim.</i> <u>1973</u> , 47, 1035.		
VARIABLES: Temperature: 225-265°C Pressure: 3.5-78.5 MPa		PREPARED BY: A. Maczynski		
EXPERIMENTAL VALUES: Solubility of water in octane				
<i>t/°C</i>	<i>p/kg cm⁻²</i>	<i>p/MPa (compiler)</i>	<i>x₂</i>	<i>g(2)/100 g sln (compiler)</i>
225	36	3.5	0.166	3.04
	100	9.8	0.137	2.44
	200	19.6	0.109	1.89
	300	29.4	0.098	1.68
	400	39.2	0.091	1.55
	500	49.0	0.088	1.50
	600	58.8	0.084	1.42
	700	68.6	0.080	1.35
800	78.5	0.075	1.26	
240	50	4.9	0.216	4.16
	100	9.8	0.193	3.63
	200	19.6	0.164	3.00
	300	29.4	0.149	2.69
	400	39.2	0.140	2.50
	500	49.0	0.132	2.34
	600	58.8	0.126	2.22
	700	68.6	0.122	2.14
800	78.5	0.117	2.05	
(continued)				
AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: The experimental technique was described in ref 1. No details reported in the paper.		SOURCE AND PURITY OF MATERIALS: (1) source not specified, chemical reagent grade; purity not specified; used as received. (2) distilled.		
		ESTIMATED ERROR: not specified.		
		REFERENCES: 1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. <i>Gazov. Prom.</i> <u>1971</u> , 4, 6.		

(1) Octane; C_8H_{18} ; [111-65-9]

Skripka, V.G.

Tr. Vses. Neftegazov. Nauch. Issled.

Inst. 1976, 61, 139-51.

(2) Water; H_2O ; [7732-18-5]

Sultanov, R.G.; Skripka, V.G.

Zh. Fiz. Khim. 1973, 47, 1035.

$t/^\circ C$	$p/kg\ cm^{-2}$	p/MPa (compiler)	x_2	$g(2)/100\ g\ sln$ (compiler)
265	75	7.4	0.412	9.95
	100	9.8	0.350	7.83
	200	19.6	0.254	5.10
	300	29.4	0.224	4.35
	400	39.2	0.207	3.95
	500	49.0	0.194	3.66
	600	58.8	0.183	3.41
	700	68.6	0.172	3.19
	800	78.5	0.163	2.98

COMPONENTS: (1) Octane; C_8H_{18} ; [111-65-9] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Krzyzanowska, T.; Szeliga, J. <i>Nafta (Katowice)</i> , <u>1978</u> , 12, 413-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of octane in water at 25°C was reported to be 0.431 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 4.31×10^{-5} g(1)/100 g sln and 6.80×10^{-8} . Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainty exists about whether the datum compiled here is independent of that of Price for the same system.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.02 mg(1)/kg(2) (standard deviation from 7-9 determinations). REFERENCES:

<p>COMPONENTS:</p> <p>(1) Octane; C₈H₁₈; [111-65-9]</p> <p>(2) Water; H₂O; [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>, <i>9</i>, 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="148 526 1105 782"> <thead> <tr> <th colspan="4" style="text-align: center;">Solubility of octane in water</th> </tr> <tr> <th style="text-align: center;">$t/^\circ\text{C}$</th> <th style="text-align: center;">mg(1)/kg sln</th> <th style="text-align: center;">$10^5\text{g(1)}/100\text{g sln}$ (compiler)</th> <th style="text-align: center;">10^7x_1 (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">15</td> <td style="text-align: center;">0.653</td> <td style="text-align: center;">6.53</td> <td style="text-align: center;">1.03</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.628</td> <td style="text-align: center;">6.28</td> <td style="text-align: center;">0.99</td> </tr> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">0.615</td> <td style="text-align: center;">6.15</td> <td style="text-align: center;">0.97</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">0.612</td> <td style="text-align: center;">6.12</td> <td style="text-align: center;">0.96</td> </tr> <tr> <td style="text-align: center;">35</td> <td style="text-align: center;">0.620</td> <td style="text-align: center;">6.20</td> <td style="text-align: center;">0.98</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 octane in water				$t/^\circ\text{C}$	mg(1)/kg sln	$10^5\text{g(1)}/100\text{g sln}$ (compiler)	10^7x_1 (compiler)	15	0.653	6.53	1.03	20	0.628	6.28	0.99	25	0.615	6.15	0.97	30	0.612	6.12	0.96	35	0.620	6.20	0.98
Solubility of octane in water																													
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<p>AUXILIARY INFORMATION</p>																													
<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, > 99.8%, 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>, <i>8</i>, 25-35.</p>																												

COMPONENTS: (1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water, H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. <i>A. I. Ch. E. J.</i> <u>1985</u> , 31, 376-84.																												
VARIABLES: Temperature: 311-553 K Pressure: 0.01-7.4 MPa	PREPARED BY: G.T. Hefter																												
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of octane in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><i>T</i>/K</th> <th style="text-align: center;"><i>p</i> /MPa</th> <th style="text-align: center;">10⁵ <i>x</i>₁</th> <th style="text-align: center;">10² g(1)/100 g sln (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">310.9</td> <td style="text-align: center;">0.0103^a</td> <td style="text-align: center;">0.012</td> <td style="text-align: center;">0.0076</td> </tr> <tr> <td style="text-align: center;">366.5</td> <td style="text-align: center;">0.117^a</td> <td style="text-align: center;">0.048</td> <td style="text-align: center;">0.030</td> </tr> <tr> <td style="text-align: center;">422.0</td> <td style="text-align: center;">0.655</td> <td style="text-align: center;">0.38</td> <td style="text-align: center;">0.24</td> </tr> <tr> <td style="text-align: center;">479.5</td> <td style="text-align: center;">2.51</td> <td style="text-align: center;">4.0</td> <td style="text-align: center;">2.5</td> </tr> <tr> <td style="text-align: center;">536.1</td> <td style="text-align: center;">7.03</td> <td style="text-align: center;">35</td> <td style="text-align: center;">22</td> </tr> <tr> <td style="text-align: center;">552.8</td> <td style="text-align: center;">8.86</td> <td style="text-align: center;">60^b</td> <td style="text-align: center;">38</td> </tr> </tbody> </table> <p>^a Estimated by the authors from pure component data ^b Above three-phase equilibrium point.</p> <p style="text-align: right;">(continued)</p>		<i>T</i> /K	<i>p</i> /MPa	10 ⁵ <i>x</i> ₁	10 ² g(1)/100 g sln (compiler)	310.9	0.0103 ^a	0.012	0.0076	366.5	0.117 ^a	0.048	0.030	422.0	0.655	0.38	0.24	479.5	2.51	4.0	2.5	536.1	7.03	35	22	552.8	8.86	60 ^b	38
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AUXILIARY INFORMATION																													
METHOD/APPARATUS/PROCEDURE: Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.	SOURCE AND PURITY OF MATERIALS: (1) Aldrich 99+ mol %; water free purity ≥ 99.9 mol %, checked by gas chromatography. (2) Distilled; no details given. ESTIMATED ERROR: soly. ± 5%, relative precision of replicate analyses. temp. not stated. press. ± 1%; type of error not stated. REFERENCES: 1. Tsonopoulos, C.; Wilson, G.M. <i>A. I. Ch. E. J.</i> <u>1983</u> , 29, 990-9.																												

(1) Octane; C₈H₁₈; [111-65-9]

(2) Water, H₂O; [7732-18-5]

(continued)

Solubility of water in octane

<i>T</i> /K	<i>p</i> /MPa	10 ² <i>x</i> ₂	<i>g</i> (2)/100 g sln (compiler)
310.9	0.0103 ^a	0.100	0.0158
366.5	0.117	0.62	0.098
422.0	0.65 ^b	3.94	0.622
477.6	- ^b	12.6	2.22
533.1	- ^b	38.7	9.05
539.1 ^c	7.41	52.7 ^c	14.9
550.4 ^d	-	54.9 ^d	16.1

^a Estimated by the authors from pure component data.

^b Not specified.

^c Three phase critical point.

^d Above three phase critical point.

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

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

$$\ln x_1 = -343.1497 + 13862.49/T + 49.24609 \ln T$$

$$\ln x_2 = -0.66037 - 7.1130 (T_p^{-1} - 1) - 0.67885 (1 - T_p)^{1/3} - 1.43381 (1 - T_p)$$

where $T_p = T/539.1$

COMPONENTS: (1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Seawater	EVALUATOR: D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982
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CRITICAL EVALUATION:

The solubility of octane (1) in seawater (2) has been reported in two works:

<u>Authors</u>	<u>Method</u>	<u>T/K</u>	<u>Salinity· g salts/kg sln</u>	<u>g(1)/100 g sln</u>
Krasnoshchekova and Gubergrits (ref 1)	GLC	298	6	2.5 x 10 ⁻⁴
Freegarde <i>et al.</i> (ref 2)	GLC	?	?	1 x 10 ⁻⁴

Because temperature and salinity are not specified, the data of Freegarde *et al.* are rejected. The value of Krasnoshchekova and Gubergrits is considered doubtful since it is greater than the tentative value for the solubility of octane in pure water at 298 K.

SOLUBILITY OF OCTANE (1) IN SEAWATER (2)
DOUBTFUL VALUE

<u>T/K</u>	<u>g salts/kg sln</u>	<u>g(1)100 g sln</u>
298	6	2.5 x 10 ⁻⁴

REFERENCES

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

COMPONENTS: (1) Octane; C_8H_{18} ; [111-65-9] (2) Seawater (composition not specified)	ORIGINAL MEASUREMENTS: Freearde, M.; Hatchard, C.G.; Parker, C.A. <i>Lab Pract.</i> <u>1971</u> , 20, 35-40.
VARIABLES: Temperature, pressure, salinity not given.	PREPARED BY: M. Kleinschmidt and D. Shaw
EXPERIMENTAL VALUES: The solubility of octane was reported to be 1.0 mg/L. The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 1.0×10^{-4} g(l)/100 g sln and 1.6×10^{-7} , assuming a solution density of 1.02 kg/L.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: None given except that analysis was done using gas chromatography.	SOURCE AND PURITY OF MATERIALS: not given. ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS: (1) Octane; C ₈ H ₁₈ ; [111-65-9] (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 octane in seawater was reported to be 2.5 x 10⁻⁴ g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 4.0 \times 10^{-7}$.</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: