

COMPONENTS: (1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.
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CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Schatzberg (ref 1)	298,313	(2) in (1)	Karl Fischer
Englin <i>et al.</i> (ref 2)	293-323	(2) in (1)	analytical
Franks (ref 3)	298	(1) in (2)	GLC
Yoshida and Yamane (ref 4)	- ^a	(1) in (2)	GLC
Skripka and Namiot (ref 5)	598 ^b	(2) in (1)	- ^a
Sutton and Calder (ref 6)	298	(1) in (2)	GLC
Skripka and Sultanov (ref 7,8)	523-598 ^b	(2) in (1)	- ^a

^a Not specified.

^b Pressure also varied.

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

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

All data on the solubility of hexadecane in water have probably been obtained at 298 K (Table 1, although Yoshida and Yamane (ref 4) did not specify their temperature). However the values are in poor agreement and no "best" value has been calculated. It may also be noted that all values are higher than the value of $\sim 2 \times 10^{-9}$ g(1)/100 g sln predicted by extrapolation of lower hydrocarbon solubilities (although whether this extrapolation remains valid for very long chain hydrocarbons is not known).

TABLE 2. Reported Solubility Values of Hexadecane (1) in Water (2)

T/K	Reported values ^a 10 ⁷ g(1)/100 g sln
298	6.3 (ref 3), 5.57 ^b (ref 4), 0.9 (ref 6)

^a No "best" value calculated due to uncertainties in data, see text.

^b Temperature not specified.

COMPONENTS: (1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986
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CRITICAL EVALUATION:

(continued)

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

The solubility of water in hexadecane at atmospheric pressure have been reported by Schatzberg (ref 1) and Englin *et al.* (ref 2) over a range of temperatures. However, agreement is poor (Table 3) and the data must be considered as very Tentative.

TABLE 3. Tentative Solubility Values of
Water (2) in Hexadecane (1)

T/K	Solubility values		
	Reported values 10 ³ g(2)/100 g sln	"Best" values (±σ _n) ^b 10 ³ g(2)/100 g sln	10 ³ x ₂
293	6.9 (ref 2)	7	0.9
298	5.4 (ref 1), 9.6 ^a (ref 2)	8 ± 2	1.0
303	12.3 (ref 2)	12	1.5
313	10.4 (ref 1), 20.9 (ref 2)	16 ± 5	2.0
323	33.2	33	4.2

^a Obtained by the Evaluator by graphical interpolation of the authors' data.

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

At higher pressures the solubility of water in hexadecane has been reported over the range 523-598 K and 1.7-78.5 MPa by Skripka *et al.* (ref 5, 7, 8). As these are the only data available under these conditions no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental values.

REFERENCES

- Schatzberg, P. *J. Phys. Chem.* **1963**, *67*, 776-9.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* **1965**, *10*, 42-6.
- Franks, F. *Nature (London)* **1966**, *210*, 87-8.
- Yoshida, F.; Yamane, T. *Biotechnol. Bioenerg.* **1971**, *13*, 691-6.
- Skripka, V.G.; Namiot, A.Yu. *Zh. Fiz. Khim.* **1974**, *48*, 782.
- Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* **1974**, *8*, 654-7.
- Skripka, V.G.; *Tr. Vses. Neftegazov Nauch Issled. Inst.* **1976**, *61*, 139-51.
- Sultanov, R.G.; Skripka, V.G. *Zh. Fiz. Khim.* **1973**, *47*, 1035.

COMPONENTS: (1) Hexadecane; $C_{16}H_{34}$; [544-76-3] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Schatzberg, P. <i>J. Phys. Chem.</i> <u>1963</u> , 67, 776-9.									
VARIABLES: Temperature: 25-40°C	PREPARED BY: M.C. Haulait-Pirson									
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in hexadecane</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;">mg(2)/kg sln</th> <th style="text-align: center;">x_2</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">54^a</td> <td style="text-align: center;">6.8×10^{-4}</td> </tr> <tr> <td style="text-align: center;">40</td> <td style="text-align: center;">104^b</td> <td style="text-align: center;">13.1×10^{-4}</td> </tr> </tbody> </table> <p>a, b See "Estimated Error"</p>		$t/^\circ C$	mg(2)/kg sln	x_2	25	54 ^a	6.8×10^{-4}	40	104 ^b	13.1×10^{-4}
$t/^\circ C$	mg(2)/kg sln	x_2								
25	54 ^a	6.8×10^{-4}								
40	104 ^b	13.1×10^{-4}								
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) Humphrey-Wilkinson, Inc.; ASIM normal cetane; 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. $\pm 0.02^\circ C$ soly. a) 0-6%; b) 0-2% (deviations from the mean) REFERENCES:									

COMPONENTS: (1) Hexadecane; $C_{16}H_{34}$; [544-76-3] (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: 20-50°C	PREPARED BY: A. Maczynski and M.C. Haulait-Pirson															
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in hexadecane</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 g sln</th> <th style="text-align: center;">$10^4 x_2$ (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.0069</td> <td style="text-align: center;">8.67</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">0.0123</td> <td style="text-align: center;">15.45</td> </tr> <tr> <td style="text-align: center;">40</td> <td style="text-align: center;">0.0209</td> <td style="text-align: center;">26.22</td> </tr> <tr> <td style="text-align: center;">50</td> <td style="text-align: center;">0.0332</td> <td style="text-align: center;">41.59</td> </tr> </tbody> </table>		$t/^\circ C$	g(2)/100 g sln	$10^4 x_2$ (compiler)	20	0.0069	8.67	30	0.0123	15.45	40	0.0209	26.22	50	0.0332	41.59
$t/^\circ C$	g(2)/100 g sln	$10^4 x_2$ (compiler)														
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40	0.0209	26.22														
50	0.0332	41.59														
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) Hexadecane; $C_{16}H_{34}$; [544-76-3] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Franks, F. <i>Nature (London)</i> <u>1966</u> , 210, 87-8.
VARIABLES: One temperature: 25°C	PREPARED BY: F. Kapuku
EXPERIMENTAL VALUES: <p>The solubility of hexadecane in water at 25°C was reported to be in mole fraction $x_1 = 5 \times 10^{-10}$.</p> <p>The corresponding mass percent calculated by the compiler is 6.3×10^{-7} g(1)/100 g sln.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator fitted to the chromatographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.</p>	SOURCE AND PURITY OF MATERIALS: (1) Fluka; purum grade; purity > 97% (chromatographic analysis). (2) not specified.
ESTIMATED ERROR: soly. \pm 12%	
REFERENCES:	

COMPONENTS: (1) Hexadecane; $C_{16}H_{34}$; [544-76-3] (2) Water, H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Yoshida, F.; Yamane, T. <i>Biotechnol. Bioeng.</i> <u>1971</u> , <i>13</i> , 691-6.
VARIABLES: One temperature: not specified	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of hexadecane in water was reported to be 5.57×10^{-9} g(l) cm^{-3} sln. With the assumption that a solution density of 1.00 g/cm, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 5.57×10^{-7} g(l)/100 g sln and 4.45×10^{-10} .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: The analytical method was used. 10 mL of (1) and 1200 mL of (2) were placed in a stoppered flask and agitated with a magnetic stirrer at a speed of 200 rpm for 9 to 24 hrs. (1) was extracted from 1000 ml of (2) with 2 mL of heptane and its concentration determined by gas chromatography using a Shimadzu equipped with hydrogen flame detectors.	SOURCE AND PURITY OF MATERIALS: not specified. ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS: (1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Skripka, V.G.; Namiot, A.Yu. <i>Zh. Fiz. Khim.</i> <u>1974</u> , 48, 782.																								
VARIABLES: One temperature: 325°C Pressure: 1.7-13.18 MPa	PREPARED BY: A. Maczynski																								
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in hexadecane at 325°C</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><u>p/kg cm⁻²</u></th> <th style="text-align: center;"><u>p/MPa (compiler)</u></th> <th style="text-align: center;"><u>x₂</u></th> <th style="text-align: center;"><u>g(2)/100 g sln (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">17.3</td> <td style="text-align: center;">1.7</td> <td style="text-align: center;">0.083</td> <td style="text-align: center;">0.71</td> </tr> <tr> <td style="text-align: center;">41.5</td> <td style="text-align: center;">4.07</td> <td style="text-align: center;">0.232</td> <td style="text-align: center;">2.34</td> </tr> <tr> <td style="text-align: center;">62.5</td> <td style="text-align: center;">6.13</td> <td style="text-align: center;">0.352</td> <td style="text-align: center;">4.14</td> </tr> <tr> <td style="text-align: center;">94.2</td> <td style="text-align: center;">9.24</td> <td style="text-align: center;">0.517</td> <td style="text-align: center;">7.85</td> </tr> <tr> <td style="text-align: center;">134.4</td> <td style="text-align: center;">13.18</td> <td style="text-align: center;">0.712</td> <td style="text-align: center;">16.43</td> </tr> </tbody> </table>		<u>p/kg cm⁻²</u>	<u>p/MPa (compiler)</u>	<u>x₂</u>	<u>g(2)/100 g sln (compiler)</u>	17.3	1.7	0.083	0.71	41.5	4.07	0.232	2.34	62.5	6.13	0.352	4.14	94.2	9.24	0.517	7.85	134.4	13.18	0.712	16.43
<u>p/kg cm⁻²</u>	<u>p/MPa (compiler)</u>	<u>x₂</u>	<u>g(2)/100 g sln (compiler)</u>																						
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AUXILIARY INFORMATION																									
METHOD/APPARATUS/PROCEDURE: Method was described in refs 1 and 2. Nothing more was reported in the paper.	SOURCE AND PURITY OF MATERIALS: (1) source not specified; CP reagent; used as received. (2) distilled. ESTIMATED ERROR: not specified. REFERENCES: 1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. <i>Neft. Khoz.</i> <u>1972</u> , 2, 57. 2. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. <i>Gazov. Delo</i> <u>1972</u> , 10, 43.																								

COMPONENTS: (1) Hexadecane; C ₁₆ H ₃₄ [544-76-3] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Sutton, C.; Calder, J.A. <i>Environ. Sci. Technol.</i> <u>1974</u> , 8, 654-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of hexadecane in water at 25°C was reported to be 0.9×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1 , of 0.7×10^{-10} .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: 175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.	SOURCE AND PURITY OF MATERIALS: (1) Analabs Inc., 99+%. (2) doubly distilled. ESTIMATED ERROR: temp. ± 0.1°C soly. ± 16% REFERENCES:

COMPONENTS: (1) Hexadecane; $C_{16}H_{34}$; [544-76-5] (2) Water; H_2O ; [7732-18-5]		ORIGINAL MEASUREMENTS: Skripka, V.G. <i>Tr. Vses. Neftegazov. Nauch. Issled. Inst.</i> 1976, 61, 139-51. Sultanov, R.G.; Skripka, V.G. <i>Zh. Fiz. Khim.</i> 1973, 47, 1035.		
VARIABLES: Temperature: 250-325°C Pressure: 3.9-78.5 MPa		PREPARED BY: A. Maczynski		
EXPERIMENTAL VALUES: Solubility of water in hexadecane				
$t/^\circ C$	$p/kg\ cm^{-2}$	p/MPa (compiler)	x_2	$g(2)/100\ g\ sln$ (compiler)
250	40	3.9	0.230	2.32
	53	5.2	0.227	2.28
	93	9.1	0.217	2.16
	100	9.8	0.216	2.14
	134	13.1	0.212	2.10
	150	14.7	0.211	2.08
	200	19.6	0.208	2.05
	300	29.4	0.197	1.91
	400	39.2	0.193	1.87
	500	49.0	0.190	1.83
	600	58.8	0.186	1.78
	700	68.6	0.182	1.74
	800	78.5	0.178	1.69
275	53	5.2	0.355	4.19
	93	9.1	0.345	4.02
	100	9.8	0.343	3.99
	134	13.1	0.336	3.87
	150	14.7	0.333	3.82
	200	19.6	0.325	3.69
	300	29.4	0.308	3.42
	400	39.2	0.290	3.15
	500	49.0	0.273	2.90
	600	58.8	0.260	2.72
700	68.6	0.250	2.58	
800	78.5	0.244	2.50	
(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> 1971, 4, 6.		

(1) Hexadecane; $C_{16}H_{34}$; [544-76-5]

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)	α_2	$g(2)/100\ g\ sln$ (compiler)
300	93	9.1	0.517	7.84
	100	9.8	0.505	7.51
	134	13.1	0.480	6.84
	150	14.7	0.469	6.56
	200	19.6	0.441	5.90
	300	29.4	0.404	5.11
	400	39.2	0.384	4.72
	500	49.0	0.366	4.39
	600	58.8	0.348	4.07
	700	68.6	0.329	3.75
800	78.5	0.310	3.45	
325	134	13.1	0.712	16.43
	150	14.7	0.643	12.53
	200	19.6	0.571	9.57
	300	29.4	0.509	7.62
	400	39.2	0.480	6.84
	500	49.0	0.466	6.49
	600	58.8	0.450	6.11
	700	68.6	0.435	5.77
	800	78.5	0.414	5.32

COMPONENTS: (1) Hexadecane; $C_{16}H_{34}$; [544-76-3] (2) Seawater	ORIGINAL MEASUREMENTS: Sutton, C.; Calder, J.A. <i>Environ. Sci. Technol.</i> <u>1974</u> , 8, 654-7.
VARIABLES: One temperature: 25°C One salinity: 35 g salts/kg sln	PREPARED BY: P.A. Meyers and D. Shaw
EXPERIMENTAL VALUES: The solubility of hexadecane in seawater was reported to be 4×10^{-8} g(l)/100 g sln and $x_1 = 3 \times 10^{-11}$.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: (1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 hrs at $25.0 \pm 0.1^\circ C$. The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.	SOURCE AND PURITY OF MATERIALS: Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with $HgCl_2$ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference. ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental error of $\pm 16\%$, yet some accommodation may have occurred due to presence of natural dissolved organic matter. REFERENCES: