

COMPONENTS: (1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3] (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 octadecane (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in octadecane.

TABLE 1. Quantitative Solubility Studies of Octadecane (1) in Water (2)

Reference	T/K	Method
Baker (ref 1)	298-353	radiotracer
Baker (ref 2)	298	radiotracer
Baker (ref 3)	298	not specified
Sutton and Calder (ref 4)	298	GLC

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

With the exception of the graphical (ref 1) and v/v data (ref 3) reported by Baker which have been excluded from consideration, all the available data (ref 2,4) are summarized in Table 2 below. The reported values are in poor agreement and both are several orders of magnitude higher than would be predicted by an extrapolation of the lower n-alkane solubilities, *viz.* $\sim 10^{-10}$ g(1)/100 g sln, although the validity of this extrapolation is unknown. Nevertheless it must be recognized that the reported values *may* be substantially in error and no "best" value has been suggested.

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

T/K	Reported values ^a
	10^7 g(1)/100 g sln $10^{10} x_1$
298	6 (ref 2), 2.1 (ref 4) 4.2 (ref 2), 1.5 (ref 4)

^a No "best" values suggested because of possible errors in data; see text.

(continued next page)

<p>COMPONENTS:</p> <p>(1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.</p>
<p>CRITICAL EVALUATION:</p> <p>(continued)</p> <p>REFERENCES</p> <ol style="list-style-type: none">1. Baker, E.G. <i>Am. Chem. Soc., Div. Petrol. Chem., Preprints - Symposia</i> <u>1956</u>, 1, No.2, 5-17.2. Baker, E.G. <i>Am. Chem. Soc., Div. Petrol. Chem., Preprints</i> <u>1958</u>, 3, No.4, C61-8.3. Baker, E.G. <i>Science</i> <u>1959</u>, 129, 871-4.4. Sutton, C.; Calder, J.A. <i>Environ. Sci. Technol.</i> <u>1974</u>, 8, 654-7.	

COMPONENTS: (1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Baker, E.G. <i>Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia</i> <u>1956</u> , 1, N°2, 5-17.
VARIABLES: Temperature: 5-80°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The authors reported that the solubility of octadecane in water increases from about 55 ppb by weight at room temperature to twice this amount at 80°C. A graph reporting the mole fraction x_1 a function of the reciprocal absolute temperature is given.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>Tritio-octadecane was used as radio-active tracer. 0.01 of active (1) was shaken with (2); the mixture was filtered through a 0.05 μm filter; 0.01 mL of filtrate was vaporized in hot oxygen and passed over CuO at 600°C; the H_2O-T_2O derived from the vaporized solvent as well as from the combusted (1) was trapped at -78°C; the melted ice was reduced by Zn and the gas was counted. Many details are given in the paper.</p>	SOURCE AND PURITY OF MATERIALS: (1) tritio-octadecane prepared by hydrogenating octadecene-1 with tritium; 100 curies of tritium were introduced per mole of (1). (2) distilled.
ESTIMATED ERROR: not specified.	
REFERENCES:	

COMPONENTS: (1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Baker, E.G. <i>Am. Chem. Soc., Div. Petrol. Chem., Preprints 1958, 3, N°4, C61-8.</i>
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of octadecane-1,2-H³ in water at 25°C was reported to be 6×10^{-9} g(1)/g(2) and that of octadecane-1-C¹⁴ 5.7×10^{-9} g(1)/g(2).</p> <p>The corresponding mass fraction and mole fraction, x_1, calculated by the compiler are 6×10^{-7} g(1)/100 g sln and 4×10^{-10}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: Tritiated or carbon-14 labeled (1) was used as tracer. The technique of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)-(2) dispersion has been described in ref 1. A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dissolved in (2).	SOURCE AND PURITY OF MATERIALS: (1) Octadecane-1,2-H ³ from Tracer Lab.; percolated through silica gel. Octadecane-1-C ¹⁴ from Nuclear Instrument and Chemical Corporation; used as received. (2) distilled. ESTIMATED ERROR: soly. 20% (standard deviation from 17 replicate runs). REFERENCES: 1. Baker, E.G. <i>Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia 1956, 1, N°2, 5.</i>

COMPONENTS: (1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Baker, E.G. <i>Science</i> <u>1959</u> , 129, 871-4.
VARIABLES: One temperature: 25°C	PREPARED BY: F. Kapuku
EXPERIMENTAL VALUES: The solubility of octadecane in water at 25°C was reported to be 7.75×10^{-7} mL(1)/100 mL(2).	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: not specified.	SOURCE AND PURITY OF MATERIALS: not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS: (1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Sutton, C.; Calder, J.A. <i>Environ. Sci. Technol.</i> <u>1974</u> , <i>8</i> , 654-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of octadecane in water at 25°C was reported to be 2.1×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1, of 1.5×10^{-10}.</p>	
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 μ m 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. $\pm 0.1^\circ C$ soly. $\pm 16\%$ REFERENCES:

COMPONENTS: (1) Octadecane; $C_{18}H_{38}$; [593-45-3] (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 octadecane in seawater was reported to be 8×10^{-8} g(l)/100 g sln and $x_1 = 5 \times 10^{-11}$.	
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: