COMPONENTS:	EVALUATOR:
(1) Nonane; C_9H_{20}; [111-84-2]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	February 1986.

CRITICAL EVALUATION: (continued)

TABLE 2. Tentative Solubility Values for Nonane (1) in Water (2)

T/K	Solubility values		
	Reported values[a] 10^5g(1)/100g sln	"Best" values ($\pm \sigma_n$)[b] 10^5g(1)/100g sln	$10^8 x_1$
293	2.89 (ref 8)	2.9	4.1
298	2.2 (ref 2), 0.71 (ref 5), 1.22 (ref 6), 2.72 (ref 8)	1.7 ± 0.8	2.4
303	1.4* (ref 6)	1.4	2.0
313	1.7* (ref 6)	1.7	2.4
323	2.2* (ref 6)	2.2	3.1
333	2.6* (ref 6)	2.6	3.7
343	3.1* (ref 6)	3.1	4.4
353	3.4* (ref 6)	3.4	4.8
363	3.7* (ref 6)	3.7	5.2
373	4.2* (ref 6)	4.2	5.9
383	8.0* (ref 6)	8.0	11
393	16* (ref 6)	16	22
403	32* (ref 6)	32	45

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the author's original data.
b Obtained by averaging where appropriate; σ_n has no statistical significance.

2. SOLUBILITY OF WATER (2) IN NONANE (1)

Only the single point data of Schatzberg (ref 1) at 298K and Benkovski *et al.* (ref 3) at 303K are available for the solubility of water in nonane and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheets for the experimental values; however, it may be noted that the data of Schatzberg (ref 1) are generally reliable.

REFERENCES

1. Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.

2. McAuliffe, C. *Science* 1969, *163*, 478-9.

3. Benkovski, V.G.; Nauruzov, M.H.; Bogoslovskaya, T.M. *Tr. Inst. Khim. Nefti Prir. Solei Alkad. Nauk Kaz. SSR* 1970, *2*, 25-32.

4. Roof, J.G. *J. Chem. Eng. Data* 1970, *15*, 301-3.

5. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-7.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Schatzberg (ref 1)	298	(2) in (1)	Karl Fischer
McAuliffe (ref 2)	298	(1) in (2)	GLC
Benkovski *et al.* (ref 3)	303	(2) in (1)	Karl Fischer
Krasnoshchekova and Gubergrits (ref 5)	298	(1) in (2)	GLC
Price (ref 6)	298-410	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 7)	298	(1) in (2)	GLC
Jonsson *et al.* (ref 8)	288,293	(1) in (2)	partition coeff.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Roof (ref 4) has also reported a three phase critical point of unspecified composition at 555K and 8.5 MPa. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF NONANE (1) IN WATER (2)

All the data available for the solubility of nonane in water are summarized in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 7) which does not appear to be independent of that of Price (ref 6) and has therefore been excluded from consideration.

At 298K, the only temperature where comparison is possible, the agreement between the various studies is poor (Table 2) and the average must be regarded as Tentative only. Interestingly, the average value of 1.7×10^{-5} g(1)/100g sln is, however, quite close to the value of 2.0×10^{-5} g(1)g sln predicted by extrapolation of the lower *n*-alkane solubilities.

At other temperatures only the data of Jonsson *et al.* (ref 8) at 293K and Price (ref 6) at 303-410K are available and thus no Critical Evaluation is possible. There are also insufficient independent data to warrant plotting.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Nonane; C_9H_{20}; [111-84-2]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	February 1986.

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

6. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.

7. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

8. Jonsson, J.A.; Vejrosta, J.; Novak, J. *Fluid Phase Equil.* 1982, *9*, 279-86.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in nonane at 25°C was reported to be 79 mg(2)/kg sln corresponding to a mole fraction, x_2, of 5.6×10^{-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) Phillips Petroleum Co.; research grade; 99.69 mole%; 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. ± 0.02°C
soly. 0-6% (deviations from the mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *Science* 1969, *163*, 478-9.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	F. Kapuku

EXPERIMENTAL VALUES:

The solubility of nonane in water at 25°C was reported to be 0.220 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.2×10^{-5} g(1)/100 g sln and 3.09×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaken for 2 minutes. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.	(1) not specified. (2) distilled.
	ESTIMATED ERROR: soly. ± 0.021 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	Benkovski, V.G.; Nauruzov, M.H.; Bogoslovskaya, T.M. *Tr. Inst. Khim. Nefti Prir. Solei Akad. Nauk Kaz. SSR* 1970, 2, 25-32.
VARIABLES:	**PREPARED BY:**
One temperature: 303 K	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in nonane at 303 K was reported to be 0.0045 g(2)/100 g sln.

The corresponding mole fraction, x_2, value calculated by compiler is 0.00032.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equal volumes of (1) and (2) were placed in a glass cylinder and periodically shaken for 6 h, then sampled and analyzed by the Karl Fischer method.	(1) source not specified; purified; purity not specified. (2) distilled.
	ESTIMATED ERROR: Not specified
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of nonane in water at 25°C was reported to be $x_1 = 1.00 \times 10^{-8}$.
The corresponding mass percent calculated by the compiler is 7.1×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) source not specified; CP reagent; purity not specified. (2) distilled.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
Temperature: 25-136.6°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of nonane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^8 x_1$ (compiler)
25.0	0.122 ± 0.007	0.0000122	1.71
69.7	0.309 ± 0.019	0.0000309	4.34
99.1	0.420 ± 0.034	0.0000420	5.90
121.3	1.70 ± 0.11	0.000170	23.9
136.6	5.07 ± 0.25	0.000507	71.2

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:	ORIGINAL MEASUREMENTS:
(1) Nonane; C_9H_{20}; [111-84-2]	Krzyzanowska, T.; Szeliga, J.
(2) Water; H_2O; [7732-18-5]	*Nafta (Katowice)*, 1978, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of nonane in water at 25°C was reported to be 0.122 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 1.22×10^{-5} g(1)/100 g sln and 1.71×10^{-8}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL 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. 0.01 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	Jonsson, J.A.; Vejrosta, J.; Novak, J. *Fluid Phase Equil.* 1982, *9*, 279-86.
VARIABLES:	**PREPARED BY:**
Temperature: 15-20°C	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of nonane (1) in water (2)

t/°C	mg(1)/kg sln	10^5g(1)/100g sln (compiler)	10^8x1 (compiler)
15	0.289	2.89	4.05
20	0.272	2.72	3.81

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).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapor concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and the entrapped (1) analyzed by gas chromatography. The method and apparatus are described in detail in ref 1.	(1) Fluka, > 99%, used as received. (2) Not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES: 1. Vejrosta, J.; Novak, J.; Jonsson, J.A. *Fluid Phase Equil.* 1982, *8*, 25-35.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C_9H_{20}; [111-84-2] (2) Seawater	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-8.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C Salinity: 6 g/kg sln	M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of nonane in seawater was reported to be 4.3×10^{-5} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 6.0 \times 10^{-8}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

SOURCE AND PURITY OF MATERIALS:

(1) "chemically pure"

(2) distilled water plus salt mixture.

ESTIMATED ERROR:

not specified.

REFERENCES: