COMPONENTS:	EVALUATOR:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	January 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,2,4-trimethylpentane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2,2,4-Trimethylpentane (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Berkengeim (ref 1)	273-313	(2) in (1)	Karl Fischer
Baker (ref 2)	unspecified	(1) in (2)	radiotracer
Englin *et al.* (ref 3)	273-323	(2) in (1)	analytical
McAuliffe (ref 4)	298	(1) in (2)	GLC
Polak and Lu (ref 5)	273,298	mutual	GLC, Karl Fischer
Budantseva *et al.* (ref 6)	293	mutual	unspecified
Price (ref 7)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 8)	298	(1) in (2)	GLC

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

1. THE SOLUBILITY OF 2,2,4-TRIMETHYLPENTANE (1) IN WATER (2)

Very few data are available for the solubility of 2,2,4-trimethylpentane in water making critical evaluation difficult. The datum of Baker (ref 2) is rejected as the temperature was not specified. All other reported values are collected in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 8) which does not appear to be independent of that of Price (ref 7) and has therefore been excluded from consideration.

At 298K where comparisons are possible, the values of McAuliffe (ref 4) and Polak and Lu (ref 5) are in reasonable agreement. The value reported by Price (ref 7) is much lower. Although Price's data for many hydrocarbons in water are normally reliable, many of his values for the higher hydrocarbons are lower than other studies. However, in the absence of confirmatory studies it is not reasonable to reject Price's value at this stage. However, it has not been included in the calculation of the "Best" values at 298K.

At other temperatures the "Best" values should be regarded with caution in the absence of confirmatory studies.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	January 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of 2,2,4-Trimethylpentane (1) in Water (2)

T/K	Solubility values		
	Reported values $10^4 g(1)/100g$ sln	"Best" values ($\pm \sigma_n$)[a] $10^4 g(1)/100g$ sln	$10^7 x_1$
273	2.46 (ref 5)	2.5	3.9
293	2 (ref 6)	2	3
298	2.44 (ref 4), 2.05 (ref 5) 1.14 (ref 7)	2.2 ± 0.2[b]	3.5[b]

[a] Obtained by averaging where appropriate; σ_n has no statistical significance.
[b] Average of data from ref 4 and 5 only, see text.

2. SOLUBILITY OF WATER (2) IN 2,2,4-TRIMETHYLPENTANE (1)

The various reported values of the solubility of water in 2,2,4-trimethylpentane are collected in Table 3 and plotted in Figure 1.

The data are generally in poor agreement and the averaged "Best" values must be regarded with caution pending further studies. Generally, for many other systems investigated by these authors, the data of Englin *et al.* (ref 3) are reliable at T < 300K but are too high at higher temperatures. Application of the van't Hoff equation to the data of Englin *et al.* and Bergengeim (ref 1) gives values of ΔH_{sln} = 41.9 and 20.1 kJ mol^{-1} and $\Delta C_{p,sln}$ = -100 and -1950 J K^{-1} mol^{-1} respectively. Comparison of these data with other systems suggests that the values of Englin *et al.* are more realistic (although probably high at T > 300K). This system clearly warrants further investigation.

TABLE 3: Tentative Values of the Solubility of Water (2) in 2,2,4-Trimethylpentane (1)

T/K	Solubility values		
	Reported values[c] $10^3 g(2)/100g$ sln	"Best" values ($\pm \sigma_n$)[a] $10^3 g(2)/100g$ sln	$10^4 x_2$
273	1.7* (ref 1), 3.1 (ref 3), 2.3 (ref 5)	2.4 ± 0.6	1.5
283	3.7 (ref 1), 5.9 (ref 3), 4.5* (ref 5)	4.7 ± 0.9	2.9
293	5.5 (ref 1), 11.5 (ref 3), 6.5* (ref 5), 7.9 (ref 6)	8 ± 2	5

(Table 3 continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,2,4-Trimethylpentane; C_8H_{18} [540-84-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	January 1986

CRITICAL EVALUATION: (continued)

Table 3 (continued)

T/K	Solubility values		
	Reported values[c] $10^3 g(2)/100g$ sln	"Best" values ($\pm \sigma_n$)[a] $10^3 g(2)/100g$ sln	$10^4 x_2$
298	6.2* (ref 1), 15.3* (ref 3), 8.0 (ref 5)	10 ± 4	6
303	7.0* (ref 1), 20.1 (ref 3)	20[b]	10[b]
313	8.0 (ref 1)		
323	53.8 (ref 3)	50[b]	30[b]

[a] Best values obtained by averaging where appropriate; σ_n has no statistical significance.
[b] Order of magnitude values only, see text.
[c] Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.

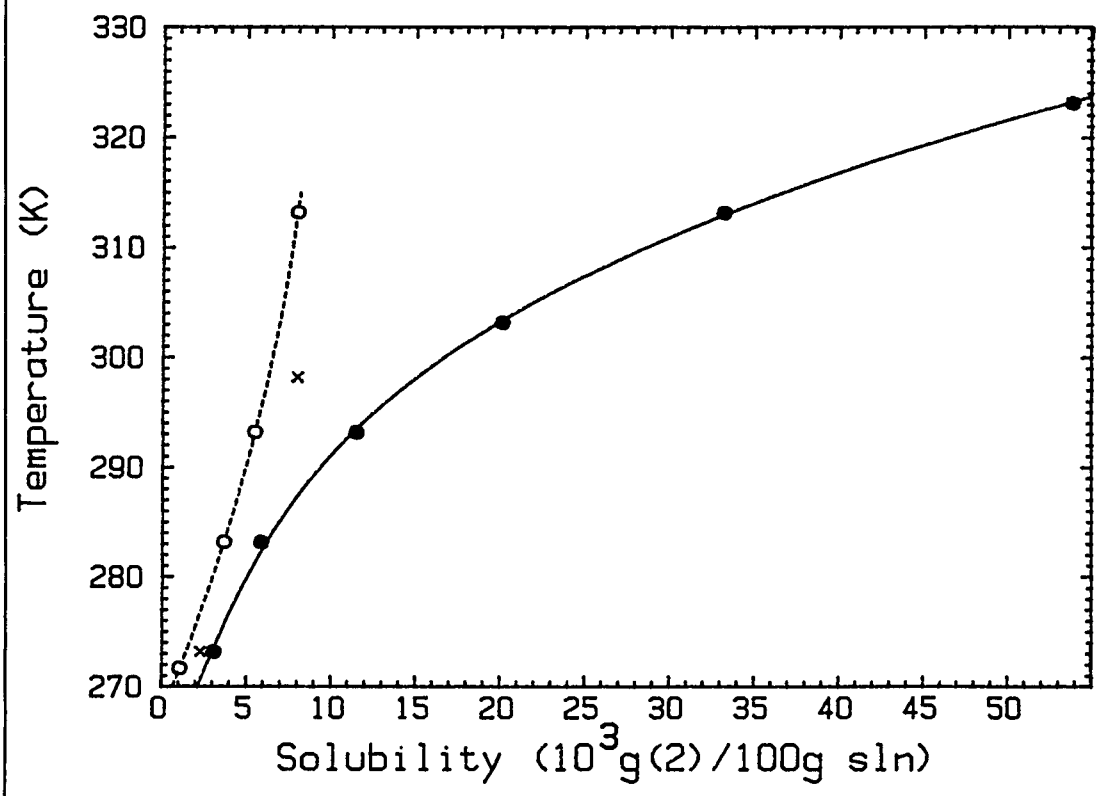

FIGURE 1. Solubility of water in 2,2,4-trimethylpentane: ref 1 (o); ref 3 (●); ref 5 (x).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	January 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Berkengeim, T.I. *Zavod. Lab.* 1941, *10*, 592-4.
2. Baker, E.G. *Geochim. Cosmochim. Acta* 1960, *19*, 309-17.
3. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
4. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
5. Polak, J.; Lu, B.C.-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
6. Budantseva, L.A.; Lesteva, T.M.; Nemtsov, M.S. *Zh. Fiz. Khim.* 1976, *50*, 1344, Deposited doc. 1976, VINITI 437-76.
7. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
8. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Marie-Claire Haulait-Pirson for comments and Dr Brian Clare for the graphics and regression analyses.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	Berkengeim, T.I. *Zavod. Lab.* 1941, *10*, 592-4.
VARIABLES:	**PREPARED BY:**
Temperature: (-1.5) - 40°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubilitv of water in 2,2,4-trimethylpentane

t/°C	g(2)/100 g sln	$10^4 x_2$ (compiler)
-1.5	0.0011	0.697
10	0.0037	2.35
20	0.0055	3.49
40	0.0080	5.07

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (2) in (1) was determined by the Karl Fischer reagent method.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; d_D^{20} 0.6947; used as received.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	Baker, E.G. *Geochim. Cosmochim. Acta* 1960, *19*, 309-17.
VARIABLES:	**PREPARED BY:**
One temperature: not specified	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water was reported to be 0.0009 mL (1) L^{-1} (2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The procedure is described in ref 1.	not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

1. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints* 1958, *3*, N°4, C61.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
VARIABLES:	**PREPARED BY:**
Temperature: 0-50°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in 2,2,4-trimethylpentane

t/°C	g(2)/100 g sln	$10^4 x_2$ (compiler)
0	0.0031	1.97
10	0.0059	3.74
20	0.0115	7.29
30	0.0201	12.74
40	0.0332	21.02
50	0.0538	34.03

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:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water at 25°C was reported to be 2.44 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is 3.85×10^{-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 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.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+% purity; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 0.12 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Nature (London)* 1963, *200*, 1092.
2. McAuliffe, C. *Am. Chem. Soc., Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
VARIABLES:	**PREPARED BY:**
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

mw = 114.23

Solubility of 2,2,4-trimethylpentane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0[a]	2.46[c]	3.88×10^{-7}
25[b]	2.05[c]	3.23×10^{-7}

Solubility of water in 2,2,4-trimethylpentane

t/°C	mg(2)/kg sln	x_2 (compiler)
0[a]	23[d]	1.46×10^{-4}
25[b]	80[e]	5.07×10^{-4}

[a-e] See "Estimated Error"

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°C; b) ± 0.01°C
soly. c) ± 4%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S. *Zh. Fiz. Khim.* 1976, *50*, 1344. *Deposited doc.* 1976, VINITI 437-76.
VARIABLES: One temperature: 20°C	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water at 20°C was reported to be $x_1 = 3 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is about 2×10^{-4} g(1)/100 g sln.

The solubility of water in 2,2,4-trimethylpentane at 20°C was reported to be $x_2 = 4.4 \times 10^{-4}$.

The corresponding mass percent value calculated by the compiler is 7.9×10^{-3} (2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Nothing specified in the paper.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water at 25°C and at system pressure was reported to be 1.14 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.14×10^{-4} g(1)/100 g sln and 1.80×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1°C soly. ± 0.02 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, 1978, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water at 25°C was reported to be 1.14 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 1.14×10^{-4} g(1)/100 g sln and 1.80×10^{-7}.

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:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. 0.04 mg(1)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES: