COMPONENTS:	EVALUATOR:
(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,3,4-trimethylpentane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2,3,4-Trimethylpentane (1) - Water (2) System

Reference	T/K	Solubility	Method
Polak and Lu (ref 1)	273,298	mutual	GLC, Karl Fischer
Price (ref 2)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 3)	298	(1) in (2)	GLC

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 in two parts.

1. THE SOLUBILITY OF 2,3,4-TRIMETHYLPENTANE (1) IN WATER (2)

All the available data on the solubility of 2,3,4-trimethylpentane in water are collected in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 3) which does not appear to be independent of that of Price (ref 2) and has thus been excluded from consideration.

At 298K, the datum of Polak and Lu (ref 1) is much higher than that reported by Price (ref 2), as for many other hydrocarbon systems investigated by these authors. In the absence of other independent studies it is not possible to prefer either datum.

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

T/K	Solubility values		
	Reported values	"Best" values ($\pm\sigma_n$)[a]	
	10^4g(1)/100g sln	10^4g(1)/100g sln	$10\ x_1$
273	2.34 (ref 1)	2.3	
298	2.30 (ref 1), 1.36 (ref 2)	1.8 ± 0.5	

[a] Obtained by simple averaging, σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.
(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: (continued)

2. THE SOLUBILITY OF WATER (2) IN 2,3,4-TRIMETHYLPENTANE (1)

As only one study of the solubility of water in 2,3,4-trimethylpentane has been reported (ref 1) no Critical Evaluation is possible. The interested user is referred to the appropriate Data Sheet for experimental values. However, it may be noted that the solubility of water in other hydrocarbons reported by Polak and Lu (ref 1) are normally reliable.

REFERENCES

1. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.

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

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3] (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:

Solubility of 2,3,4-trimethylpentane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0[a]	2.34[c]	3.69×10^{-7}
25[b]	2.30[c]	3.62×10^{-7}

Solubility of water in 2,3,4-trimethylpentane

t/°C	mg(2)/kg sln	x_2 (compiler)
0[a]	20[d]	1.27×10^{-4}
25[b]	74[e]	4.69×10^{-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) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3] (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 2,3,4-trimethylpentane in water at 25°C and at system pressure was reported to be 1.36 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.36 x 10^{-4} g(1)/100 g sln and 2.14 x 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. ± 0.03 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3]	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 2,3,4-trimethylpentane in water at 25°C was reported to be 1.36 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 1.36×10^{-4} g(1)/100 g sln and 2.14×10^{-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:

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. 0.05 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES: