COMPONENTS:

(1) 3-Methylpentane; C_6H_{14}; [96-14-0]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.
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November 1984

CRITICAL EVALUATION:

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

TABLE 1: Quantitative Solubility Studies of the 3-Methylpentane (1) - Water (2) System

Reference	*T*/K	Solubility	Method
McAuliffe (ref 1)	298	(1) in (2)	GLC
Polak and Lu (ref 2)	273,298	mutual	GLC, Karl Fischer
Price (ref 3)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 4)	298	(1) in (2)	GLC
Rudakov and Lutsyk (ref 5)	298	(1) in (2)	partition coefficient

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 3-METHYLPENTANE (1) IN WATER (2)

Of the data reported for the solubility of 3-methylpentane in water (Table 1), the datum of Krzyzanowska and Szeliga (ref 4) has been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 3). The 298K datum of Polak and Lu (ref 2) is much higher (*ca*. 30% relative) than all other reported values (ref 1, 3, 5). Furthermore, the value at 273K, as with other hydrocarbons investigated by these authors, shows an unusually large increase over the value at 298K. Thus the data of Polak and Lu (ref 2) are rejected. All the remaining data (all at 298K) are listed in Table 2).

TABLE 2: Recommended (*R*) Value for the Solubility of 3-Methylpentane (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values (± σ_n)^a	
	10^3g(1)/100g sln	10^3g(1)/100g sln	10^5x_1
298	1.28 (ref 1), 1.31 (ref 3), 1.29 (ref 5)	1.29 ± 0.01 (*R*)	2.70 (*R*)

[a] "Best" values obtained by averaging; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 3-Methylpentane; C_6H_{14}; [96-14-0] (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. November 1984

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) in 3-METHYLPENTANE (1)

The solubility of water in 3-methylpentane has been reported only by Polak and Lu (ref 2) and thus no Critical Evaluation can be made. The interested user is referred to the relevant Data Sheet for solubility values. However, it can be noted that the data of Polak and Lu are generally close to "Recommended" values in well characterized systems.

REFERENCES

1. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
2. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
3. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
4. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.
5. Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* 1979, *53*, 1298-1300.

COMPONENTS:

(1) 3-Methylpentane; C_6H_{14}; [96-14-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylpentane in water at 25°C was reported to be 12.8 mg (1)/kg sln (0.00128 g(1)/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler, is 2.68×10^{-6}.

The same value is also reported in ref 1.

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 K

soly. 0.6 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:

(1) 3-Methylpentane; C_6H_{14}; [96-14-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 3-methylpentane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0^a	21.5^c	4.49×10^{-6}
25^b	17.9^c	3.74×10^{-6}

Solubility of water in 3-methylpentane

t/°C	mg(2)/kg sln	x_2 (compiler)
0^a	23^d	1.10×10^{-4}
25^b	94^e	4.50×10^{-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 K; b) ± 0.01 K
soly. c) ± 1.7%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:

(1) 3-Methylpentane; C_6H_{14};
[96-14-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull.
1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylpentane in water at 25°C and at system pressure was reported to be 13.1 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00131 g(1)/100 g sln and 2.74×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1 K
soly. ± 0.4 mg(1)/kg(2)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylpentane; C_6H_{14}; [96-14-0] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylpentane in water at 25°C was reported to be 13.10 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.00131 g(1)/100 g sln and 2.74 x 10^{-6}.

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:

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

REFERENCES:

COMPONENTS:

(1) 3-Methylpentane; C_6H_{14}; [96-14-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rudakov, E.S.; Lutsyk, A.I.

Zh. Fiz. Khim. 1979, *53*, 1298-1300.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported the partition coefficient α of 3-methylpentane between the gas and aqueous phase. $\alpha = 68 \pm 4$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25°C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of p (where p is the vapor pressure in mm of Hg) is taken from ref 1. $p = 189.8$ mm of Hg and $\log C_g = \log p - 4.269 = -1.99$ expressed in moles per liter. Therefore $C_s = 1.50 \times 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is 0.0013 g(1)/100 g sln and the corresponding mole fraction, x_1, is 2.7×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. ± 10% (estimated by the compiler)

REFERENCES:

1. Hine, J.; Mooker, P.K. *J. Org. Chem.* 1975, *4*, 292.