COMPONENTS:	EVALUATOR:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (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:

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

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

Reference	T/K	Solubility	Method
Guseva and Parnov (ref 1)	335-487	(1) in (2)	synthetic?
Englin et al. (ref 2)	283-303	(2) in (1)	analytical
McAuliffe (ref 3)	298	(1) in (2)	GLC
Price (ref 4)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 5)	298	(1) in (2)	GLC
Rudakov and Lutsyk (ref 6)	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 METHYLCYCLOPENTANE (1) IN WATER (2)

The solubility data for methylcyclopentane in water at 298K are listed in Table 2. The datum of Krzyzanowska and Szeliga (ref 5) has been excluded from consideration as it does not appear to be independent of that of Price (ref 4). The high temperature data of Guseva and Parnov (ref 1) presumably made in sealed tubes are rejected because of inadequate specification of system conditions (especially pressure). All other data are given in Table 2.

TABLE 2: Recommended Value of the Solubility of Methylcyclopentane (1) in Water (2)

T/K	Solubility values		
	Reported values $10^3 g(1)/100g$ sln	"Best" values ($\pm \sigma_n$)^a $10^3 g(1)/100g$ sln	$10^6 x_1$
298	4.2 (ref 3), 4.18 (ref 4), 4.5 (ref 6)	4.3 ± 0.1	9.2

a Obtained by averaging, σ_n has no statistical significance.

COMPONENTS:	EVALUATOR:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (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 METHYLCYCLOPENTANE (1)

The solubility of water in methylcyclopentane has been reported in only one publication: Englin *et al.* (ref 2), and thus no Critical Evaluation can be given. However, it should be noted that in well characterized systems (e.g. benzene-water), the data of Englin *et al.* are generally reliable at lower temperatures but are higher than "Recommended" values when $T > 300K$. The interested user is referred to the appropriate data sheet for the original values.

REFERENCES

1.   Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1964, *19*, 77-8.

2.   Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.

3.   McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1967-75.

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

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

6.   Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* 1979, *53*, 1298-1300.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1964</u>, *19*, 77-8.

VARIABLES:	PREPARED BY:
Temperature: 61.5-214°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of methylcyclopentane in water

$t/°C$	g(1)/100 g(2)	g(1)/100 g sln (compiler)	$10^4 x_1$ (compiler)
61.5	0.0229	0.0229	0.490
146	0.155	0.155	3.31
184	0.457	0.457	9.76
214	1.479	1.457	31.20

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.	(1) not specified. (2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1963</u>, *18*, 76.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H_2O; [7732-18-5]	*Khim. Tekhnol. Topl. Masel* <u>1965</u>, *10*, 42-6.

VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in methylcyclopentane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
10	0.073	3.4
20	0.0131	6.12
30	0.0205	9.58

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of methylcyclopentane in water at 25°C was reported to
be 42 mg (1)/kg sln.
The corresponding mole fraction, x_1, calculated by the compiler,
is 9.0×10^{-6}.
The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 1.6 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092. 2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of methylcyclopentane in water at 25°C and at system pressure was reported to be 41.8 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00418 g(1)/100 g sln and 8.95×10^{-6}.

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 or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 1 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (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 methylcyclopentane in water at 25°C was reported
to be 41.8 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated
by compiler are 0.00418 g(1)/100 g sln and 8.95×10^{-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:	SOURCE AND PURITY OF MATERIALS:
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. 1.05 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Water; H_2O; [7732-18-5]	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 methylcyclopentane between the gas and aqueous phase. $\alpha = 14 \pm 1$. $\alpha = C_g/C_s$ 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. $p = 137.5$ mm of Hg and $\log C_g = \log p - 4.269 = -2.13$ expressed in moles per liter. Therefore $C_s = 5.29 \times 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is 0.0045 g(1)/100 g sln and the corresponding mole fraction, x_1, is 9.6×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Sodium chloride; NaCl; [7647-14-5] (3) 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 Salinity: 1-360 g(2)/kg sln	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of Methylcyclopentane in Aqueous NaCl

Salinity g(2)/kg sln	Mass Percent g(1)/100 g sln	Mole fraction $10^6 x_1$ (compilers)
1.002	0.00380	8.14
10.000	0.00363	7.82
34.472[a]	0.00292	6.40
50.030	0.00270	5.98
125.100	0.00127	2.94
199.900	0.000572	1.38
279.800	0.000336	0.847
358.700	0.000189	0.495

[a]Artificial seawater, composition not specified but probably
similar to ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Details given in source. (1) was equilibrated with NaCl solution for one month. An aliquot was analyzed directly by gas chromatography.	(1) commercial, 99 + % pure

	ESTIMATED ERROR:
	Temperature ± 1 K Solubility ± 10 relative %

	REFERENCES:
	1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* __1940__, *3*, 135.