

COMPONENTS:		EVALUATOR:	
(1) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2]		M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.	
(2) Water; H ₂ O; [7732-18-5]		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 methylcyclohexane (1) and water (2) have been reported in the publications listed in Table 1.			
<u>TABLE 1: Quantitative Solubility Studies of the Methylcyclohexane (1) - Water (2) System</u>			
Reference	T/K	Solubility	Method
Guseva and Parnov (ref 1)	341-488	(1) in (2)	synthetic?
Englin <i>et al.</i> (ref 2)	283-303	(2) in (1)	analytical
McAuliffe (ref 3)	298	(1) in (2)	GLC
Price (ref 4)	298-423	(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
<p>The original data in 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.</p> <p>1. THE SOLUBILITY OF METHYLCYCLOHEXANE (1) IN WATER (2)</p> <p>At 298K the various solubility values (ref 3, 4, 6) are in good agreement (Table 2). The datum of Krzyzanowska and Szeliga (ref 5) has been excluded from consideration because it does not appear to be independent of that of Price (ref 4).</p> <p>At other temperatures the values of Guseva and Parnov (ref 1), probably obtained in sealed tubes at unspecified pressures, are almost an order of magnitude larger than those of Price (ref 4) and are thus rejected. All other data are listed in Table 2 and plotted in Figure 1.</p> <p>Roof (ref 7) has reported a critical end point at 572.2K and 3.47 MPa.</p>			
(continued next page)			

COMPONENTS: (1) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: 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
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CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (R) and Tentative Values of
 the Solubility of Methylcyclohexane (1) in Water (2)

T/K	Solubility values		
	Reported values ^a 10 ³ g(1)/100g sln	"Best" values (± σ _n) 10 ³ g(1)/100g sln	10 ⁶ x ₁
298	1.4 (ref 3), 1.60 (ref 4), 1.53 (ref 6)	1.51 ± 0.08 (R)	2.94 (R)
303	1.7* (ref 4)	1.7	3.1
313	1.8* (ref 4)	1.8	3.3
323	1.9* (ref 4)	1.9	3.5
343	2.2* (ref 4)	2.2	4.0
363	2.9* (ref 4)	2.9	5.3
383	5.2* (ref 4)	5.2	9.6
403	18.8* (ref 4)	11	20
423	24.5* (ref 4)	25	46

^a Values marked with an asterisk (*) have been obtained by the Evaluators by graphical interpolation of the original data.

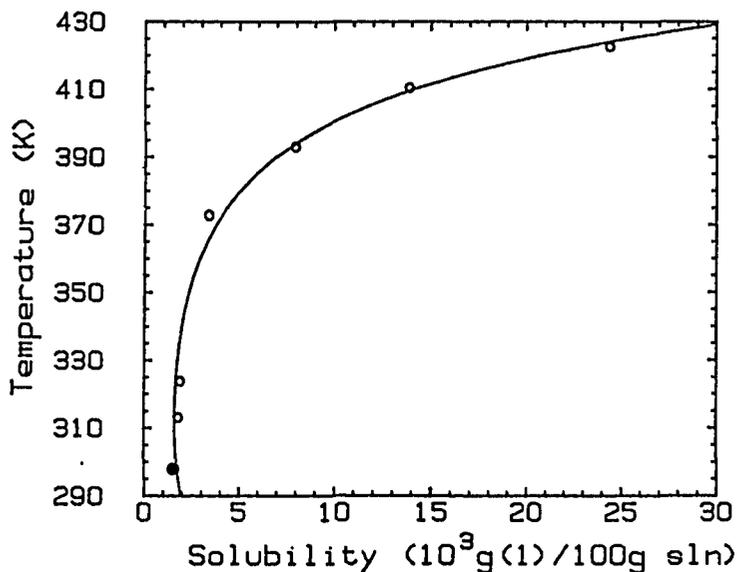


FIGURE 1. Solubility of methylcyclohexane in water : ref 4 (o); average of ref 3, 4 & 6 (●).

(continued next page)

COMPONENTS: (1) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: 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 METHYLCYCLOHEXANE (1) The solubility of water in methylcyclohexane has been reported only by Englin <i>et al.</i> (ref 2) and so no critical evaluation can be made. The interested user is referred to the relevant Data Sheet for solubility values. However, it should be noted that the data of Englin <i>et al.</i> are generally reliable at lower temperatures but are high when $T > 300\text{K}$. REFERENCES 1. Guseva, A.N.; Parnov, E.I. <i>Vestn. Mosk. Univ. Khim.</i> <u>1964</u> , <i>19</i> , 77-8. 2. Englin, B.A.; Plate, A.F.; Tugolikhov, V.M.; Pryanishnikova, M.A. <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u> , <i>10</i> , 42-6. 3. McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u> , <i>70</i> , 1267-75. 4. Price, L.C. <i>Am. Assoc. Petrol. Geol. Bull.</i> <u>1976</u> , <i>60</i> , 213-44. 5. Krzyzanowska, T.; Szeliga, J. <i>Nafta (Katowice)</i> <u>1978</u> , <i>34</i> , 413-7. 6. Rudakov, E.S.; Lutsyk, A.I. <i>Zh. Fiz. Khim.</i> <u>1979</u> , <i>53</i> , 1298-1300. 7. Roof, J.G.; <i>J. Chem. Eng. Data</i> <u>1970</u> , <i>15</i> , 301-3. ACKNOWLEDGEMENT The Evaluators thank Dr Brian Clare for the graphics.	

COMPONENTS: (1) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Guseva, A.N.; Parnov, E.I. <i>Vestn. Mosk. Univ. Khim.</i> <u>1964</u> , 19, 77-8.																				
VARIABLES: Temperature: 68-215°C	PREPARED BY: M.C. Haulait-Pirson																				
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of methylcyclohexane in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>g(l)/100 g(2)</u></th> <th style="text-align: center;"><u>g(l)/100 g sln (compiler)</u></th> <th style="text-align: center;"><u>10⁴x₁ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">68</td> <td style="text-align: center;">0.011</td> <td style="text-align: center;">0.011</td> <td style="text-align: center;">0.20</td> </tr> <tr> <td style="text-align: center;">120.5</td> <td style="text-align: center;">0.0363</td> <td style="text-align: center;">0.0363</td> <td style="text-align: center;">0.67</td> </tr> <tr> <td style="text-align: center;">157.5</td> <td style="text-align: center;">0.0933</td> <td style="text-align: center;">0.0933</td> <td style="text-align: center;">1.71</td> </tr> <tr> <td style="text-align: center;">215</td> <td style="text-align: center;">0.759</td> <td style="text-align: center;">0.759</td> <td style="text-align: center;">13.90</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>g(l)/100 g(2)</u>	<u>g(l)/100 g sln (compiler)</u>	<u>10⁴x₁ (compiler)</u>	68	0.011	0.011	0.20	120.5	0.0363	0.0363	0.67	157.5	0.0933	0.0933	1.71	215	0.759	0.759	13.90
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AUXILIARY INFORMATION																					
METHOD/APPARATUS/PROCEDURE: Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: not specified. REFERENCES: 1. Guseva, A.N.; Parnov, E.I. <i>Vestn. Mosk. Univ. Khim.</i> <u>1963</u> , 18, 76.																				

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VARIABLES: Temperature: 10-30°C	PREPARED BY: A. Maczynski and M.C. Haulait-Pirson												
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in methylcyclohexane</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;">$t/^\circ C$</th> <th style="text-align: center;">$g(2)/100\ g\ sln$</th> <th style="text-align: center;">$10^4 x_2$ (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">10</td> <td style="text-align: center;">0.0061</td> <td style="text-align: center;">3.33</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.0116</td> <td style="text-align: center;">6.32</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">0.0179</td> <td style="text-align: center;">9.75</td> </tr> </tbody> </table>		$t/^\circ C$	$g(2)/100\ g\ sln$	$10^4 x_2$ (compiler)	10	0.0061	3.33	20	0.0116	6.32	30	0.0179	9.75
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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: (1) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u> , <i>70</i> , 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of methylcyclohexane in water at 25°C was reported to be 14 mg (1)/kg sln (0.0014 g(1)/100 g sln).</p> <p>The corresponding mole fraction, x_1, calculated by the compiler, is 2.6×10^{-6}.</p> <p>The same value is also reported in refs 1 and 2.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>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.</p>	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled. ESTIMATED ERROR: temp. \pm 1.5 K soly. 1.2 mg (1)/kg sln (standard deviation from mean) REFERENCES: 1. McAuliffe, C. <i>Nature (London)</i> <u>1963</u> , <i>200</i> , 1092. 2. McAuliffe, C. <i>Am. Chem. Soc. Div. Petrol. Chem.</i> <u>1964</u> , <i>9</i> , 275.

COMPONENTS: (1) Methylcyclohexane; C_7H_{14} ; [108-87-2] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Price, L.C. <i>Am. Assoc. Petrol. Geol. Bull.</i> <u>1976, 60, 213-44.</u>																																
VARIABLES: Temperature: 25-149.5°C	PREPARED BY: F. Kapuku																																
EXPERIMENTAL VALUES: Solubility of methylcyclohexane in water at system pressure <table border="1" data-bbox="220 546 1163 889"> <thead> <tr> <th>$t/^\circ C$</th> <th>mg(1)/kg(2)</th> <th>g(1)/100 g sln (compiler)</th> <th>$10^6 x_1$ (compiler)</th> </tr> </thead> <tbody> <tr> <td>25.0</td> <td>16.0 ± 0.2</td> <td>0.00160</td> <td>2.9</td> </tr> <tr> <td>40.1</td> <td>18.0 ± 0.6</td> <td>0.00180</td> <td>3.3</td> </tr> <tr> <td>55.7</td> <td>18.9 ± 0.5</td> <td>0.00189</td> <td>3.5</td> </tr> <tr> <td>99.1</td> <td>33.8 ± 1.0</td> <td>0.00338</td> <td>6.2</td> </tr> <tr> <td>120.0</td> <td>79.5 ± 2.2</td> <td>0.00795</td> <td>14.6</td> </tr> <tr> <td>137.3</td> <td>139.0 ± 8.0</td> <td>0.01390</td> <td>25.5</td> </tr> <tr> <td>149.5</td> <td>244.0 ± 10.0</td> <td>0.02440</td> <td>44.8</td> </tr> </tbody> </table>		$t/^\circ C$	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)	25.0	16.0 ± 0.2	0.00160	2.9	40.1	18.0 ± 0.6	0.00180	3.3	55.7	18.9 ± 0.5	0.00189	3.5	99.1	33.8 ± 1.0	0.00338	6.2	120.0	79.5 ± 2.2	0.00795	14.6	137.3	139.0 ± 8.0	0.01390	25.5	149.5	244.0 ± 10.0	0.02440	44.8
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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 K soly. range of values given above REFERENCES:																																

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VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of methylcyclohexane in water at 25°C was reported to be 16.0 mg(1)/kg(2).</p> <p>The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0016 g(1)/100 g sln and 2.93×10^{-6}.</p> <p>Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainty exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>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.</p>	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: soly. 0.5 mg(1)/kg(2) (standard deviation from 7-9 determinations) REFERENCES:

COMPONENTS: (1) Methylcyclohexane; C_7H_{14} ; [108-87-2] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Rudakov, E.S.; Lutsyk, A.I. <i>Zh. Fiz. Khim.</i> <u>1979</u> , <i>53</i> , 1298-1300.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The authors reported the partition coefficient α of methylcyclohexane between the gas and aqueous phase. $\alpha = 16 \pm 1$. $\alpha = C_g/C_s$ 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).</p> <p>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. $p = 46.33$ mm of Hg and $\log C_g = \log p - 4.269 = -2.60$ expressed in moles per liter. Therefore $C_s = 1.56 \times 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is $0.0015 \text{ g(1)/100 g sln}$ and the corresponding mole fraction, x_1, is 2.7×10^{-6}.</p>	
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. $\pm 10\%$ (estimated by the compiler) REFERENCES: 1. Hine, J.; Mooker, P.K. <i>J. Org. Chem.</i> <u>1975</u> , <i>4</i> , 292.