

COMPONENTS: (1) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985
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CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Black <i>et al.</i> (ref 1)	279-295	(2) in (1)	radiotracer
Englin <i>et al.</i> (ref 2)	273-293	(2) in (1)	analytical
McAuliffe (ref 3)	298	(1) in (2)	GLC
Pavlova <i>et al.</i> (ref 4)	293-333	mutual	GLC, Karl Fischer
Polak and Lu (ref 5)	273,298	mutual	GLC, Karl Fischer
Price (ref 6)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 7)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

In the Tables which follow, solubilities obtained by the Evaluator by graphical interpolation of original measurements in the Data Sheets are indicated by an asterisk (*). "Best" values have been obtained, where appropriate, by simple averaging. Uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than error limits.

For convenience, further discussion of this system will be divided into two parts.

1. THE SOLUBILITY OF 2-METHYLBUTANE (1) IN WATER (2)

The solubility data for 2-methylbutane in water are listed in Table 2 and are also plotted in Figure 1. The data of Krzyzanowska and Szeliga (ref 7) have been excluded from this Evaluation as they do not appear to be independent of those reported by Price (ref 6).

At 298K, where comparison amongst independent values is possible, agreement is excellent. This gives added confidence to the values at other temperatures. A possible exception may be the value of Polak and Lu (ref 5) at 273K which appears a little high (even though some increase in solubility of hydrocarbons in water is usually observed as the temperature approaches 273K, e.g. the benzene-water system). (continued next page)

COMPONENTS: (1) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985.
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CRITICAL EVALUATION: (continued)

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

<i>T</i> /K	Solubility values		
	Reported values 10 ³ g(1)/100g sln	"Best" values (± σ _n) 10 ³ g(1)/100g sln	10 ⁵ x ₁
273	7.24 (ref 5)	7.2 ^a	1.8 ^a
293	4.69 (ref 4)	4.7	1.2
298	4.78 (ref 3), 4.86* (ref 4), 4.96 (ref 5), 4.8 (ref 6)	4.85 ± 0.07 (<i>R</i>)	1.21 (<i>R</i>)
303	5.06* (ref 4)	5.1	
313	5.77 (ref 4)	5.8	1.4
323	7.01 (ref 4)	7.0	1.8
333	7.93 (ref 4)	7.9	2.0

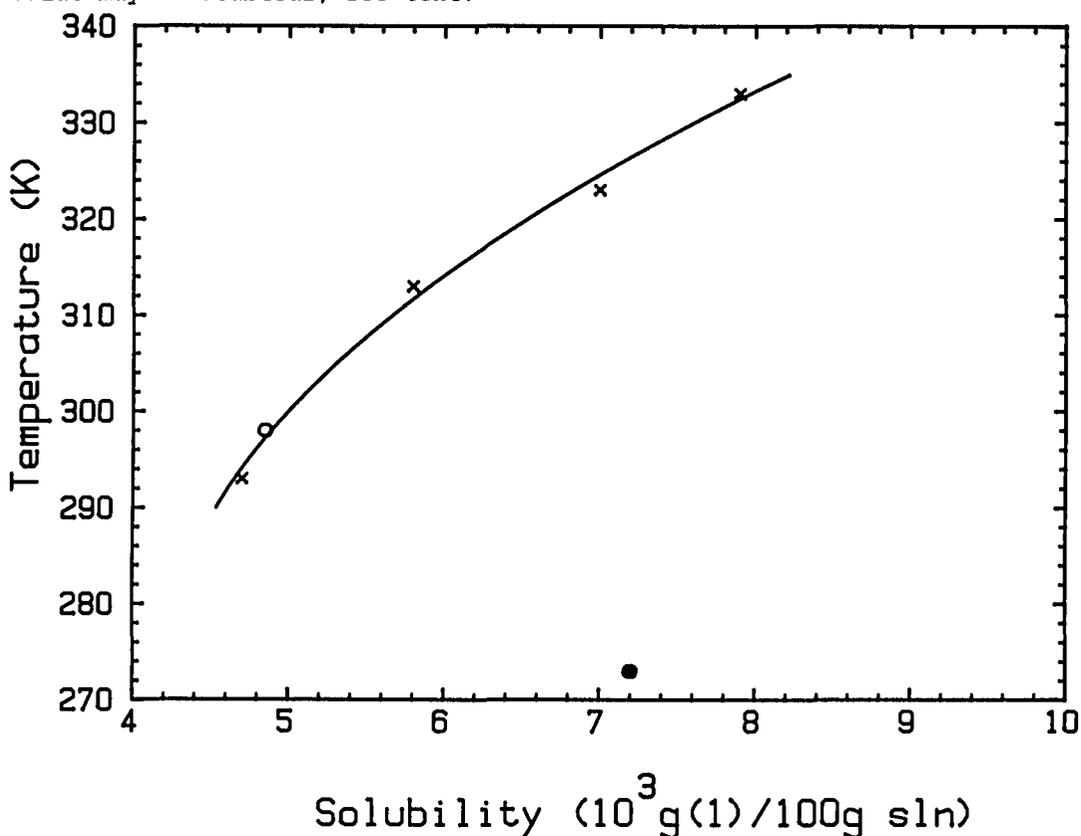
^aValue may be doubtful, see text.

FIGURE 1. Solubility of 2-methylbutane in water: ref 4 (x); average of
ref 3-6 (o); ref 5 (●), but see text.

(continued next page)

COMPONENTS: (1) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985
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CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN 2-METHYLBUTANE (1)

The solubility data for water in 2-methylbutane are listed in Table 3 and plotted in Figure 2. In general the reported values are in reasonable agreement. The only exception appears to be the data of Pavlova *et al.* (ref 4) which are higher than other values. Although there are insufficient independent data to justify outright rejection of the values of Pavlova *et al.* at this stage, nevertheless, their data have not been used in determining "best" values (Table 3) and should be regarded with caution.

TABLE 3: Tentative Values of the Solubility of
Water (2) in 2-Methylbutane (1)

T/K	Solubility values		
	Reported values 10 ³ g(2)/100g sln	"Best" values (± σ _n) ^a 10 ³ g(2)/100g sln	10 ⁴ x ₂
273	3.2 (ref 2), 2.8 (ref 5)	3.0 ± 0.2	1.2
278	4.3* (ref 1)	4.3	1.7
283	5.2* (ref 1), 5.9 (ref 2)	5.5 ± 0.4	2.2
288	6.5* (ref 1)	6.5	2.6
293	9.2* (ref 1), 11.2 (ref 2), 16.0 (ref 4)	10 ± 1	4
298	18* (ref 4), 9.6 (ref 5)	10	4
303	20* (ref 4)		
313	25.7 (ref 4)		
323	40* (ref 4)		
333	58.5 (ref 4)		

^aData from ref 4 not included in calculation of "best" values, see text.

(continued next page)

COMPONENTS:

(1) 2-Methylbutane; C_5H_{12} ; [78-78-4](2) Water; H_2O ; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical
and Physical Sciences, Murdoch
University, Perth, W.A., Australia.
July 1985

CRITICAL EVALUATION: (continued)

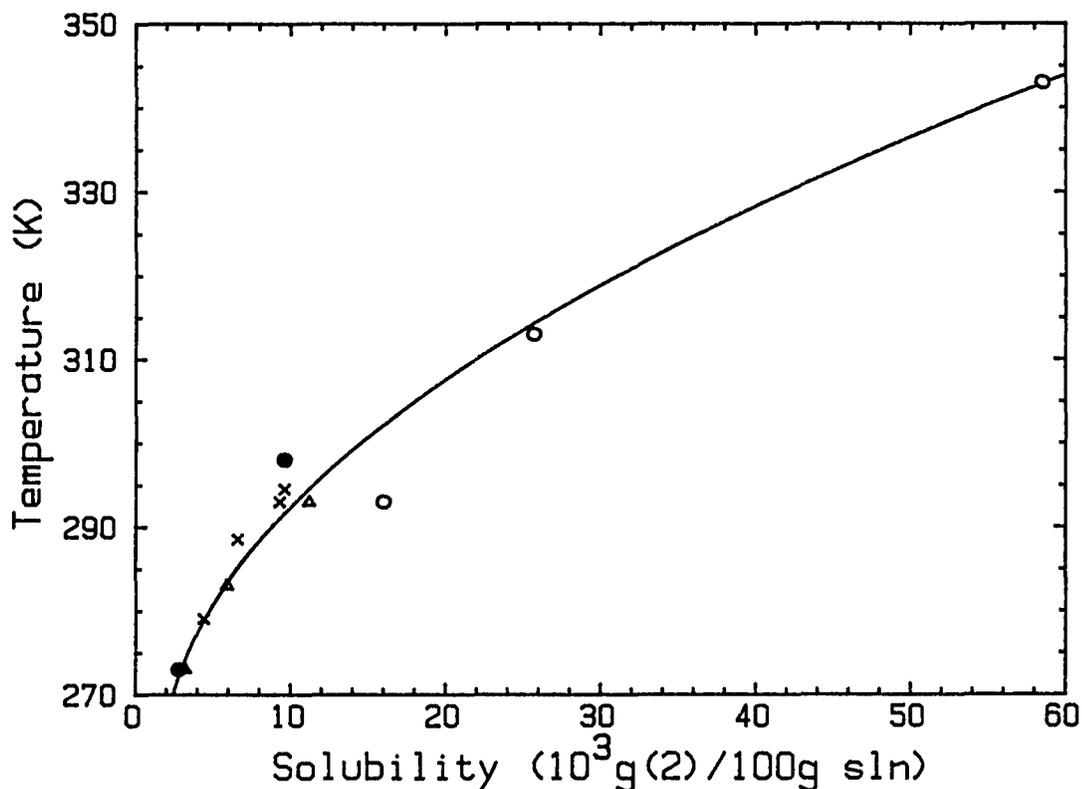


FIGURE 2. Solubility of water in 2-methylbutane: ref 1 (x); ref 2 (Δ); ref 4 (o), ref 5 (●).

REFERENCES

- Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* 1948, *16*, 537-43.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Maseł* 1965, *10*, 42-6.
- McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
- Pavlova, S.P.; Pavlov, S.Yu.; Serafimov, L.A.; Kofman, L.S. *Promyshlennost. Sinteticheskovo Kauchuka* 1966, *3*, 18-20.
- Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
- Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
- Krzyżanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

COMPONENTS: (1) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Black, C.; Joris, G.G.; Taylor, H.S. <i>J. Chem. Phys.</i> <u>1948</u> , <i>16</i> , 537-43.																																								
VARIABLES: Temperature: 6-21.8°C	PREPARED BY: M.C. Haulait-Pirson																																								
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in 2-methylbutane at a total saturation pressure of 1 atm</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;">t/°C</th> <th style="text-align: center;">g(2)/100 g(1)</th> <th style="text-align: center;">g(2)/100 g sln (compiler)</th> <th style="text-align: center;">10⁴x₂ (compiler)</th> </tr> </thead> <tbody> <tr> <td>15.3</td> <td>0.0066*</td> <td>0.0066</td> <td>2.6</td> </tr> <tr> <td>21.3</td> <td>0.0096*</td> <td>0.0096</td> <td>3.8</td> </tr> <tr> <td>21.8</td> <td>0.0097*</td> <td>0.0097</td> <td>3.9</td> </tr> <tr> <td rowspan="3">6.0</td> <td>0.00443</td> <td>0.00443</td> <td>1.78</td> </tr> <tr> <td>0.00433</td> <td>0.00433</td> <td>1.74</td> </tr> <tr> <td>0.00440</td> <td>0.00440</td> <td>1.76</td> </tr> <tr> <td rowspan="3">20.0</td> <td>0.00940</td> <td>0.00940</td> <td>3.76</td> </tr> <tr> <td>0.00902</td> <td>0.00902</td> <td>3.61</td> </tr> <tr> <td>0.00942</td> <td>0.00942</td> <td>7.77</td> </tr> <tr> <td>20.5</td> <td>0.01001</td> <td>0.01001</td> <td>4.02</td> </tr> </tbody> </table> <p>*Determinations made in glass apparatus</p>		t/°C	g(2)/100 g(1)	g(2)/100 g sln (compiler)	10 ⁴ x ₂ (compiler)	15.3	0.0066*	0.0066	2.6	21.3	0.0096*	0.0096	3.8	21.8	0.0097*	0.0097	3.9	6.0	0.00443	0.00443	1.78	0.00433	0.00433	1.74	0.00440	0.00440	1.76	20.0	0.00940	0.00940	3.76	0.00902	0.00902	3.61	0.00942	0.00942	7.77	20.5	0.01001	0.01001	4.02
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AUXILIARY INFORMATION																																									
METHOD/APPARATUS/PROCEDURE: The method described in ref 1 in which tritium oxide acts as a tracer, was used. Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred in the counter through equilibration with ethanol vapor.	SOURCE AND PURITY OF MATERIALS: (1) Ohio State University under an American Petroleum Institute project; purity not specified; used as received. (2) not specified.																																								
ESTIMATED ERROR: soly. a few percent (type of error not specified).																																									
REFERENCES: 1. Joris, G.G.; Taylor, H.S. <i>J. Chem. Phys.</i> <u>1948</u> , <i>16</i> , 45.																																									

COMPONENTS: (1) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u> , 10, 42-6.												
VARIABLES: Temperature: 0-20°C	PREPARED BY: A. Maczynski and M.C. Haulait-Pirson												
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of water in 2-methylbutane</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>g(2)/100 g sln</u></th> <th style="text-align: center;"><u>10⁴x₂</u> (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0</td> <td style="text-align: center;">0.0032</td> <td style="text-align: center;">1.28</td> </tr> <tr> <td style="text-align: center;">10</td> <td style="text-align: center;">0.0059</td> <td style="text-align: center;">2.37</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.0112</td> <td style="text-align: center;">4.49</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>g(2)/100 g sln</u>	<u>10⁴x₂</u> (compiler)	0	0.0032	1.28	10	0.0059	2.37	20	0.0112	4.49
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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: (1) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4] (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 2-methylbutane in water at 25°C was reported to be 47.8 mg (l)/kg sln, (0.0478 g(l)/100 g sln). The corresponding mole fraction, x_1, calculated by the compiler, is 1.19×10^{-5}. 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. 1.6 mg (l)/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) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Pavlova, S.P.; Pavlov, S.Yu.; Serafimov, L.A.; Kofman, L.S. <i>Promyshlennost. Sinteticheskogo Kauchuka</i> <u>1966</u> , 3, 18-20.																											
VARIABLES: Temperature: 20-60°C	PREPARED BY: A. Maczynski																											
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of 2-methylbutane in water</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>10⁵x₁</u></th> <th style="text-align: center;"><u>g(1)/100 g sln (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">1.17</td> <td style="text-align: center;">0.00469</td> </tr> <tr> <td style="text-align: center;">40</td> <td style="text-align: center;">1.44</td> <td style="text-align: center;">0.00577</td> </tr> <tr> <td style="text-align: center;">50</td> <td style="text-align: center;">1.75</td> <td style="text-align: center;">0.00701</td> </tr> <tr> <td style="text-align: center;">60</td> <td style="text-align: center;">1.98</td> <td style="text-align: center;">0.00793</td> </tr> </tbody> </table> <p style="text-align: center;">Solubility of water in 2-methylbutane</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>10³x₂</u></th> <th style="text-align: center;"><u>g(2)/100 g sln (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.64</td> <td style="text-align: center;">0.0160</td> </tr> <tr> <td style="text-align: center;">40</td> <td style="text-align: center;">1.03</td> <td style="text-align: center;">0.0257</td> </tr> <tr> <td style="text-align: center;">60</td> <td style="text-align: center;">2.34</td> <td style="text-align: center;">0.0585</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>10⁵x₁</u>	<u>g(1)/100 g sln (compiler)</u>	20	1.17	0.00469	40	1.44	0.00577	50	1.75	0.00701	60	1.98	0.00793	<u>t/°C</u>	<u>10³x₂</u>	<u>g(2)/100 g sln (compiler)</u>	20	0.64	0.0160	40	1.03	0.0257	60	2.34	0.0585
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METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	SOURCE AND PURITY OF MATERIALS: (1) source not specified; better than 99.7 wt%. (2) doubly distilled. ESTIMATED ERROR: temp. ± 0.1 K REFERENCES:																											

COMPONENTS: (1) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Polak, J.; Lu, B.C-Y. <i>Can. J. Chem.</i> <u>1973</u> , 51, 4018-23.																		
VARIABLES: Temperature: 0-25°C	PREPARED BY: M.C. Haulait-Pirson																		
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of 2-methylbutane 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>mg(1)/kg sln</u></th> <th style="text-align: center;"><u>x₁ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0^a</td> <td style="text-align: center;">72.4^c</td> <td style="text-align: center;">1.81 × 10⁻⁵</td> </tr> <tr> <td style="text-align: center;">25^b</td> <td style="text-align: center;">49.6^c</td> <td style="text-align: center;">1.24 × 10⁻⁵</td> </tr> </tbody> </table> <p style="text-align: center;">Solubility of water in 2-methylbutane</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>mg(2)/kg sln</u></th> <th style="text-align: center;"><u>x₂ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0^a</td> <td style="text-align: center;">28^d</td> <td style="text-align: center;">1.12 × 10⁻⁴</td> </tr> <tr> <td style="text-align: center;">25^b</td> <td style="text-align: center;">96^e</td> <td style="text-align: center;">3.85 × 10⁻⁴</td> </tr> </tbody> </table> <p>a-e see "ESTIMATED ERROR"</p>		<u>t/°C</u>	<u>mg(1)/kg sln</u>	<u>x₁ (compiler)</u>	0 ^a	72.4 ^c	1.81 × 10 ⁻⁵	25 ^b	49.6 ^c	1.24 × 10 ⁻⁵	<u>t/°C</u>	<u>mg(2)/kg sln</u>	<u>x₂ (compiler)</u>	0 ^a	28 ^d	1.12 × 10 ⁻⁴	25 ^b	96 ^e	3.85 × 10 ⁻⁴
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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) 2-Methylbutane; C_5H_{12} ; [78-78-4] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Price, L.C. <i>Am. Assoc. Petrol. Geol. Bull.</i> <u>1976</u> , 60, 213-44.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of 2-methylbutane in water at 25°C and at system pressure was reported to be 48 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.0048 g(1)/100 g sln and 1.20×10^{-5} .	
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 Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 1 mg(1)/kg(2)
	REFERENCES:

COMPONENTS: (1) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Krzyzanowska, T.; Szeliga, J. <i>Nafta Katowice</i> <u>1978</u> , 12, 413-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of 2-methylbutane in water at 25°C was reported to be 48 mg(1)/kg(2).</p> <p>The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0048 g(1)/100 g sln and 1.2×10^{-5}.</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. 1.44 mg(1)/kg(2) (standard deviation from 7-9 determinations)	
REFERENCES:	