

COMPONENTS: (1) 2-Methyl-1,3-butadiene; C ₅ H ₈ ; [78-79-5] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Australia. November 1984.
---	--

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
McAuliffe (ref 1)	298	(1) in (2)	GLC
Pavlova <i>et al.</i> (ref 2)	293-533	mutual	GLC, Karl Fischer

As only one study of the solubility of (2) in (1) has been reported (ref 2), no Critical Evaluation of those data can be made. The interested user is referred to the relevant data sheet for experimental values.

The reported values of the solubility of (1) in (2) are listed in Table 2 and plotted in Figure 1. The agreement at 298 K between the value of McAuliffe (ref 1) and the interpolated value of Pavlova *et al.* (ref 2) is reasonable so the "Best" values in Table 2 may be considered "Tentative", subject to further studies.

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

T/K	Solubility values		
	Reported values g(1)/100g sln	"Best" values ($\pm \sigma_n$) g(1)/100g sln	$10^4 x_1$
293	0.0545 (ref 2)	0.054	1.44
298	0.0642 (ref 1), 0.0572 ^a (ref 2)	0.061 \pm 0.004 ^b	1.61 ^b
313	0.0665 (ref 2)	0.066	1.76
323	0.0761 (ref 2)	0.076	2.01
333	0.0867 (ref 2)	0.087	2.29

^a Graphically interpolated by the Evaluator.

^b "Best" value obtained by averaging; σ_n has no statistical significance.

(continued next page)

COMPONENTS:

- (1) 2-Methyl-1,3-butadiene; C_5H_8 ;
[78-79-5]
(2) Water; H_2O ; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical
and Physical Sciences, Murdoch
University, Perth, Australia.
November 1984.

CRITICAL EVALUATION: (continued)

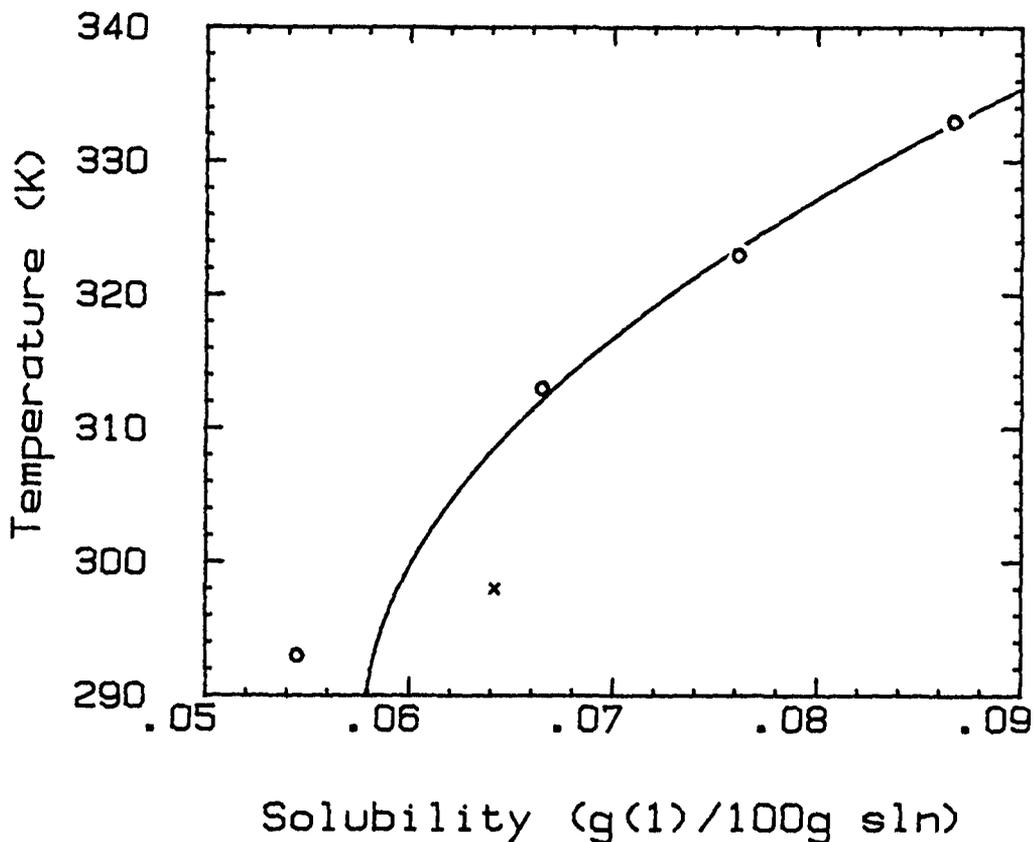


FIGURE 1. Solubility of 2-methyl-1,3-butadiene (1) in water: ref 1 (x);
ref 2 (o).

REFERENCES

1. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
2. Pavlova, S.P.; Pavlov, S.Yu.; Serafimov, L.A.; Kofman, L.S. *Promyshlennost. Sinteticheskogo Kauchuka* 1966, *3*, 18-20.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS: (1) 2-Methyl-1,3-butadiene; C_5H_8 ; [78-79-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u> , 70, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES: <p>The solubility of 2-methyl-1,3-butadiene in water at 25°C was reported to be $642 \text{ g(1)/10}^6 \text{ g(2)}$.</p> <p>The corresponding mass percent and mole fraction, x_1, calculated by the compilers are $0.0642 \text{ g(1)/100 g sln}$ and 1.70×10^{-4}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>In a 250-mL 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. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.</p>	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. $\pm 1.5K$ soly. $10 \text{ g(1)/10}^6 \text{ g(2)}$ (standard deviation of mean) REFERENCES:

COMPONENTS: (1) 2-Methyl-1,3-butadiene; C_5H_8 ; [78-79-5] (2) Water; H_2O ; [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-methyl-1,3-butadiene in water</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;">$10^4 x_1$</th> <th style="text-align: center;">$g(1)/100\text{ g sln}$ (compiler)</th> </tr> </thead> <tbody> <tr><td style="text-align: center;">20</td><td style="text-align: center;">1.441</td><td style="text-align: center;">0.05448</td></tr> <tr><td style="text-align: center;">40</td><td style="text-align: center;">1.758</td><td style="text-align: center;">0.06646</td></tr> <tr><td style="text-align: center;">50</td><td style="text-align: center;">2.013</td><td style="text-align: center;">0.07609</td></tr> <tr><td style="text-align: center;">60</td><td style="text-align: center;">2.294</td><td style="text-align: center;">0.08671</td></tr> </tbody> </table> <p style="text-align: center;">Solubility of water in 2-methyl-1,3-butadiene</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;">$10^3 x_2$</th> <th style="text-align: center;">$g(2)/100\text{ g sln}$ (compiler)</th> </tr> </thead> <tbody> <tr><td style="text-align: center;">20</td><td style="text-align: center;">2.26</td><td style="text-align: center;">0.0598</td></tr> <tr><td style="text-align: center;">40</td><td style="text-align: center;">3.58</td><td style="text-align: center;">0.0949</td></tr> <tr><td style="text-align: center;">60</td><td style="text-align: center;">5.53</td><td style="text-align: center;">0.1468</td></tr> </tbody> </table>		$t/^\circ C$	$10^4 x_1$	$g(1)/100\text{ g sln}$ (compiler)	20	1.441	0.05448	40	1.758	0.06646	50	2.013	0.07609	60	2.294	0.08671	$t/^\circ C$	$10^3 x_2$	$g(2)/100\text{ g sln}$ (compiler)	20	2.26	0.0598	40	3.58	0.0949	60	5.53	0.1468
$t/^\circ C$	$10^4 x_1$	$g(1)/100\text{ g sln}$ (compiler)																										
20	1.441	0.05448																										
40	1.758	0.06646																										
50	2.013	0.07609																										
60	2.294	0.08671																										
$t/^\circ C$	$10^3 x_2$	$g(2)/100\text{ g sln}$ (compiler)																										
20	2.26	0.0598																										
40	3.58	0.0949																										
60	5.53	0.1468																										
AUXILIARY INFORMATION																												
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. \pm 0.1K REFERENCES:																											