

<p>COMPONENTS:</p> <p>(1) Ethylcyclohexane; C<sub>8</sub>H<sub>16</sub>; [1678-91-7]</p> <p>(2) Water; H<sub>2</sub>O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.</p> <p>May 1986.</p>
--	--

## CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Guseva and Parnov (ref 1)	352-486	(1) in (2)	unspecified <sup>a</sup>
Heidman <i>et al.</i> (ref 2)	311-561	mutual	GLC, Karl Fischer

<sup>a</sup> Probably using the synthetic method.

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system is in two parts.

#### 1. SOLUBILITY OF ETHYLCYCLOHEXANE (1) IN WATER (2)

This system almost certainly exhibits type III phase behaviour (see introductory material at the beginning of this volume). The phase diagram is similar to that of ethylbenzene and water.

The solubility of ethylcyclohexane in water at elevated temperatures and system pressures along the three phase equilibrium line have been investigated by Guseva and Parnov (ref 1) and Heidman *et al.* (ref 2). Their results are summarized in Table 2 and plotted in Figure 1. The agreement is very poor. However, it may be noted (ref 1) that the values reported by Guseva and Parnov at higher temperatures approach those of cyclohexane which is unreasonable. It may also be noted that the data of Guseva and Parnov often differ markedly from Recommended values in other systems. The data of Heidman *et al.* are thus considered Tentative.

Heidman *et al.* report a three phase critical end point at  $561.4 \pm 0.6$  K,  $9.93 \pm 0.04$  MPa and  $x_1 = 3.35 \times 10^{-3}$  (2.05 g(1)/100g sln, Evaluator).

(continued next page)

## COMPONENTS:

(1) Ethylcyclohexane;  $C_8H_{16}$ ;  
[1678-91-7](2) Water;  $H_2O$ ; [7732-18-5]

## EVALUATOR:

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

May 1986.

## CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Solubility Values for Ethylcyclohexane (1) in  
Water (2) at the Three-Phase Equilibrium Pressure

T/K	Solubility values		
	Reported values <sup>a</sup> $10^2 g(1)/100g\ sln$	"Best" values <sup>b</sup> $10^2 g(1)/100g\ sln$	$10^4 x_1$
313	0.066 (ref 2)	0.07	0.01
323	0.074 (ref 2)	0.07	0.011
333	0.086 (ref 2)	0.07	0.014
343	0.10 (ref 2)	0.10	0.016
353	0.5 (ref 1), 0.13 (ref 2)	0.13	0.020
363	0.8 (ref 1), 0.16 (ref 2)	0.16	0.026
373	1.3 (ref 1), 0.21 (ref 2)	0.21	0.034
393	2.2 (ref 1), 0.55 (ref 2)	0.55	0.088
413	3.7 (ref 1), 0.95 (ref 2)	0.95	0.15
433	6.5 (ref 1), 1.6 (ref 2)	1.6	0.26
453	16.0 (ref 1), 2.8 (ref 2)	2.8	0.45
473	27.0 (ref 1), 5.5 (ref 2)	5.5	0.9
493	16 (ref 2)	16	2.2
513	34 (ref 2)	34	5.2
533	65 (ref 2)	65	10.4
553	150 (ref 2)	150	24.0

<sup>a</sup> All data obtained by graphical or algebraic interpolation by the Evaluator of the authors' original data.

<sup>b</sup> Rounded values from ref 2; data from ref 1 not included in "Best" values, see text.

(continued next page)

## COMPONENTS:

- (1) Ethylcyclohexane;  $C_8H_{16}$ ;  
[1678-91-7]  
(2) Water;  $H_2O$ ; [7732-18-5]

## EVALUATOR:

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

May 1986.

## CRITICAL EVALUATION: (continued)

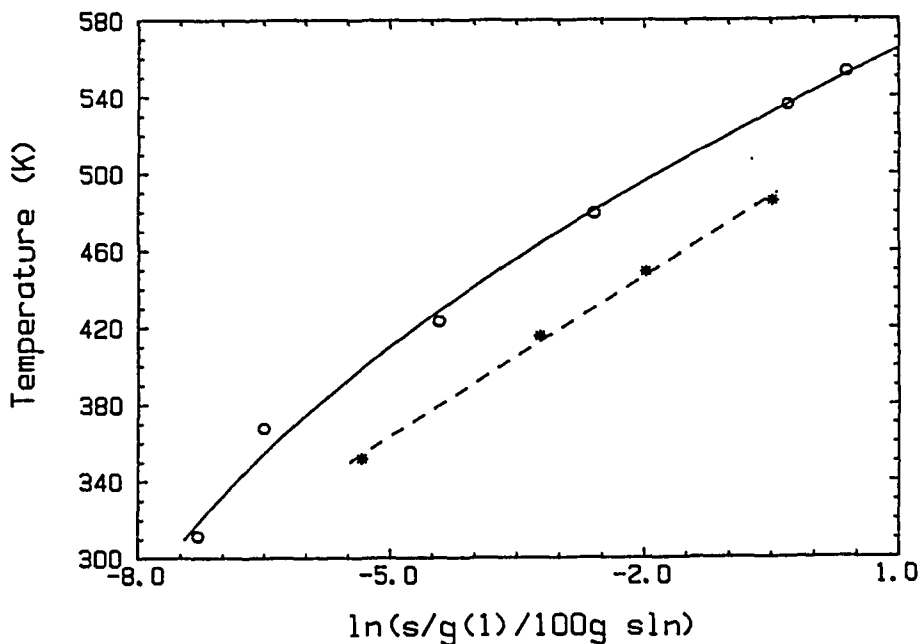


FIGURE 1. Solubility of ethylcyclohexane in water at elevated temperatures and equilibrium pressures: ref 1 (x); ref 2 (o).

## 2. SOLUBILITY OF WATER (2) IN ETHYLCYCLOHEXANE (1)

As only the data of Heidman *et al.* (ref 2) are available on the solubility of water in ethylcyclohexane (Table 1) no Critical Evaluation of water is possible. The interested user is referred to the appropriate Data Sheet for the experimental values.

## REFERENCES

- Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1964, *12*, 77-8.
- Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. *A.I.Ch.E.J.* 1985, *31*, 376-84.

## ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics and Dr Colin Young for his comments on the phase behaviour of this system.

<b>COMPONENTS:</b>  (1) Ethylcyclohexane; $C_8H_{16}$ ; [1678-91-7]  (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Guseva, A.N.; Parnov, E.I.  <i>Vestn. Mosk. Univ. Khim.</i> <u>1964</u> , 19, 77-8.																				
<b>VARIABLES:</b>  Temperature: 79-213°C	<b>PREPARED BY:</b>  M.C. Haulait-Pirson																				
<b>EXPERIMENTAL VALUES:</b>  <p style="text-align: center;">Solubility of ethylcyclohexane 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(1)/100 g(2)</u></th> <th style="text-align: center;"><u>g(1)/100 g sln (compiler)</u></th> <th style="text-align: center;"><u><math>10^4 x_1</math> (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">79</td> <td style="text-align: center;">0.0048</td> <td style="text-align: center;">0.0048</td> <td style="text-align: center;">0.077</td> </tr> <tr> <td style="text-align: center;">142.5</td> <td style="text-align: center;">0.0398</td> <td style="text-align: center;">0.0398</td> <td style="text-align: center;">0.639</td> </tr> <tr> <td style="text-align: center;">176</td> <td style="text-align: center;">0.138</td> <td style="text-align: center;">0.138</td> <td style="text-align: center;">2.22</td> </tr> <tr> <td style="text-align: center;">213</td> <td style="text-align: center;">0.66</td> <td style="text-align: center;">0.62</td> <td style="text-align: center;">9.96</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>g(1)/100 g(2)</u>	<u>g(1)/100 g sln (compiler)</u>	<u><math>10^4 x_1</math> (compiler)</u>	79	0.0048	0.0048	0.077	142.5	0.0398	0.0398	0.639	176	0.138	0.138	2.22	213	0.66	0.62	9.96
<u>t/°C</u>	<u>g(1)/100 g(2)</u>	<u>g(1)/100 g sln (compiler)</u>	<u><math>10^4 x_1</math> (compiler)</u>																		
79	0.0048	0.0048	0.077																		
142.5	0.0398	0.0398	0.639																		
176	0.138	0.138	2.22																		
213	0.66	0.62	9.96																		
<b>AUXILIARY INFORMATION</b>																					
<b>METHOD/APPARATUS/PROCEDURE:</b>  Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) not specified. (2) not specified.  <b>ESTIMATED ERROR:</b> not specified.  <b>REFERENCES:</b> 1. Guseva, A.N.; Parnov, E.I. <i>Vestn. Mosk. Univ. Khim.</i> <u>1963</u> , 18, 76.																				

<p>COMPONENTS:</p> <p>(1) Ethylcyclohexane; C<sub>8</sub>H<sub>16</sub>; [1678-91-7]</p> <p>(2) Water, H<sub>2</sub>O; [7732-18-5]</p>	<p>ORIGINAL MEASUREMENTS:</p> <p>Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. <i>A. I. Ch. E. J.</i> <u>1985</u>, <i>31</i>, 376-84.</p>																												
<p>VARIABLES:</p> <p>Temperature: 311-561 K</p> <p>Pressure: 0.01-9.9 MPa</p>	<p>PREPARED BY:</p> <p>G.T. Hefter</p>																												
<p>EXPERIMENTAL VALUES:</p> <p style="text-align: center;">Solubility of ethylcyclohexane in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><i>T</i>/K</th> <th style="text-align: center;"><i>p</i> /MPa</th> <th style="text-align: center;">10<sup>4</sup> <i>x</i><sub>1</sub></th> <th style="text-align: center;">10<sup>2</sup> g(1)/100 g sln (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">311.5</td> <td style="text-align: center;">--<sup>a</sup></td> <td style="text-align: center;">0.011</td> <td style="text-align: center;">0.068</td> </tr> <tr> <td style="text-align: center;">367.6</td> <td style="text-align: center;">0.117</td> <td style="text-align: center;">0.024</td> <td style="text-align: center;">0.15</td> </tr> <tr> <td style="text-align: center;">423.4</td> <td style="text-align: center;">0.647</td> <td style="text-align: center;">0.20</td> <td style="text-align: center;">1.2</td> </tr> <tr> <td style="text-align: center;">479.5</td> <td style="text-align: center;">2.36</td> <td style="text-align: center;">1.21</td> <td style="text-align: center;">7.5</td> </tr> <tr> <td style="text-align: center;">536.1</td> <td style="text-align: center;">6.69</td> <td style="text-align: center;">11.8</td> <td style="text-align: center;">73</td> </tr> <tr> <td style="text-align: center;">552.8</td> <td style="text-align: center;">8.83</td> <td style="text-align: center;">23.7</td> <td style="text-align: center;">146</td> </tr> </tbody> </table> <p><sup>a</sup> Not specified.</p> <p style="text-align: right;">(continued)</p>		<i>T</i> /K	<i>p</i> /MPa	10 <sup>4</sup> <i>x</i> <sub>1</sub>	10 <sup>2</sup> g(1)/100 g sln (compiler)	311.5	-- <sup>a</sup>	0.011	0.068	367.6	0.117	0.024	0.15	423.4	0.647	0.20	1.2	479.5	2.36	1.21	7.5	536.1	6.69	11.8	73	552.8	8.83	23.7	146
<i>T</i> /K	<i>p</i> /MPa	10 <sup>4</sup> <i>x</i> <sub>1</sub>	10 <sup>2</sup> g(1)/100 g sln (compiler)																										
311.5	-- <sup>a</sup>	0.011	0.068																										
367.6	0.117	0.024	0.15																										
423.4	0.647	0.20	1.2																										
479.5	2.36	1.21	7.5																										
536.1	6.69	11.8	73																										
552.8	8.83	23.7	146																										
<p>AUXILIARY INFORMATION</p>																													
<p>METHOD/APPARATUS/PROCEDURE:</p> <p>Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p>(1) Aldrich 99+ mol %; water free purity ≥ 99.9 mol %, checked by gas chromatography.</p> <p>(2) Distilled; no details given.</p> <p>ESTIMATED ERROR:</p> <p>soly. ± 5%, relative precision of replicate analyses.</p> <p>temp. not stated.</p> <p>press. ± 1%; type of error not stated.</p> <p>REFERENCES:</p> <p>1. Tsonopoulos, C.; Wilson, G.M. <i>A. I. Ch. E. J.</i> <u>1983</u>, <i>29</i>, 990-9.</p>																												

(1) Ethylcyclohexane,  $C_8H_{16}$ ; [1678-91-7]

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

(continued)

Solubility of water in ethylcyclohexane

$T/K$	$p /MPa$	$10^2 x_2$	$g(2)/100 g sln$ (compiler)
310.9	0.0099 <sup>a</sup>	0.081	0.0130
367.6	0.117	0.65	0.104
423.4	0.647	3.0	0.48
479.5	2.36	10.7	1.89
536.1	6.69	29.0	6.15
552.8	8.83	41.4	10.2
561.4 <sup>b</sup>	9.93 <sup>b</sup>	60.3 <sup>b</sup>	19.6

<sup>a</sup> Estimated by the authors from pure component data.

<sup>b</sup> Three phase critical point.

The three phase critical point was reported to be  $561.4 \pm 0.6 K$ ,  $9.93 \pm 0.04 MPa$  and  $x_1 = 3.35 \times 10^{-3}$  (1.05 g(1)/100 g sln, compiler).

The authors also report an equation which fits their own and related literature data over the range 273-561 K, *viz.*

$$\ln x_1 = -334.2468 + 14105.21/T + 47.93102 \ln T$$

$$\ln x_2 = -0.50980 - 7.4603 (T_r^{-1} - 1) - 0.67885 (1 - T_r)^{1/3} + 0.44796 (1 - T_r)$$

where  $T_r = T/561.4$