

## COMPONENTS:

- (1) 1,3-Dibromobenzene;  $C_6H_4Br_2$ ;  
[108-36-1]
- (2) Water,  $H_2O$ ; [7732-18-5]

## EVALUATOR:

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## CRITICAL EVALUATION:

The solubility of 1,3-dibromobenzene in water was reported by Hine et al. (1) at 308.15 K and by Yalkowsky et al. (2) at 298.15 K. Considering the small temperature difference of 10 degrees between the two measurements, one can judge that the data show a significant discrepancy.

The reported experimental errors  $\pm 5.6\%$  (1) and  $\pm 10\%$  (2) are probably greater than the authors anticipated. A careful study of the experimental procedures described in both articles reveals no obvious shortcomings. Despite the long time allowed for equilibrium by Hine et al., their measurements resulted in a lower solubility value than that obtained by Yalkowsky et al. The most likely explanation for the discrepancy could be attributed to the analytical determinations used.

It is well known that the solubility curve for halogenated benzenes in water has a positive slope above room temperature. However, the two measured points reported are against this trend, that is, the values decrease with rising temperature. In order to choose between the two solubility data values, use was made of the theoretical relationship between the molar solubilities and the molar volumes of the solutes at 298.15 K as described in the Introduction. The following solubility value for 1,3-dibromobenzene in water is tentative:

T/K	$10^4 \text{ mol}(1)/\text{dm}^3$	$10^2 \text{ g}(1)/\text{kg}$	$10^6 x(1)$
298.15	2.70	6.40	4.89

## REFERENCES

- Hine, J.; Haworth, H. W.; Ramsay, O. B. *J. Am. Chem. Soc.* 1963, *85*(10), 1473-6.
- Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18*(4), 351-3.

<b>COMPONENTS:</b> (1) 1,3-Dibromobenzene; $C_6H_4Br_2$ ; [108-36-1] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Hine, J.; Haworth, H. W.; Ramsay, O. B. <i>J. Am. Chem. Soc.</i> <u>1963</u> , <i>85</i> (10), 1473-6.								
<b>VARIABLES:</b> One temperature	<b>PREPARED BY:</b> A. L. Horvath								
<b>EXPERIMENTAL VALUES:</b>  <table border="0" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;"><math>t/^\circ C</math></th> <th style="text-align: left;"><math>10^2 g(1)/dm^3</math> <sup>a</sup></th> <th style="text-align: left;"><math>10^4 mol(1)/dm^3</math> <sup>b</sup></th> <th style="text-align: left;"><math>10^6 x(1)</math> <sup>c</sup></th> </tr> </thead> <tbody> <tr> <td style="text-align: left;">30.0</td> <td style="text-align: left;">6.747</td> <td style="text-align: left;">2.86</td> <td style="text-align: left;">5.184</td> </tr> </tbody> </table> <p>a. Calculated by F. W. Getzen.          b. Reported.          c. Calculated by compiler.</p>		$t/^\circ C$	$10^2 g(1)/dm^3$ <sup>a</sup>	$10^4 mol(1)/dm^3$ <sup>b</sup>	$10^6 x(1)$ <sup>c</sup>	30.0	6.747	2.86	5.184
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30.0	6.747	2.86	5.184						
<b>AUXILIARY INFORMATION</b>									
<b>METHOD/APPARATUS/PROCEDURE:</b> An excess of 1,3-dibromobenzene was added to a 4 ml of water in an ampoule which was then sealed. The sealed ampoule was rotated in a constant temperature water bath for a week to establish saturation. The 1,3-dibromobenzene solubility was determined by ultraviolet spectrophotometric measurements using a Beckman DU spectrophotometer.	<b>SOURCE AND PURITY OF MATERIALS:</b> $C_6H_4Br_2$ : Eastman Kodak Co.; redistilled before use. $H_2O$ : Not specified.  <b>ESTIMATED ERROR:</b> Solubility: $\pm 5.6\%$ S.D. Temperature: $\pm 0.1$ K.  <b>REFERENCES:</b>								

<b>COMPONENTS:</b> (1) 1,3-Dibromobenzene; $C_6H_4Br_2$ ; [108-36-1] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. <i>Ind. Eng. Chem. Fundam.</i> <u>1979</u> , <i>18</i> (4), 351-3.								
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25	9.838	4.17	7.536						
<b>AUXILIARY INFORMATION</b>									
<b>METHOD/APPARATUS/PROCEDURE:</b> A small excess of 1,3-dibromobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The saturated filtrate solution was diluted and assayed spectrophotometrically. Two independent determinations were carried out.	<b>SOURCE AND PURITY OF MATERIALS:</b> $C_6H_4Br_2$ : Aldrich commercial grade, used as received. $H_2O$ : Deionized.  <b>ESTIMATED ERROR:</b> Solubility: $\pm 10\%$ . Temperature: $\pm 1$ K.  <b>REFERENCES:</b>								