

## Correlation of the Aqueous Solubilities of Benzene Polycarboxylic Acids Using a Modified Regular Solution Model

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The modified SHFH model, based on the regular solution theory coupled with a Flory-Huggins entropy term, was applied to correlate the solubilities of benzene polycarboxylic acids in water within wide temperature ranges. The literature data were correlated by optimizing internal energies and molar volumes of the benzene polycarboxylic acids, which were treated as species dependent constants and functions of the density of water. It was found that the reported experimental data were well represented by the present proposed model with a simple expression, rather high accuracy and fewer parameters. The aqueous solubility of benzene polycarboxylic acids in the literature were explored for 1009 data points within the temperature range 273-463 K for 25 systems, and calculations were well correlated, with the total absolute average deviation ( $\delta_{AAD}$ ) of 6.76%. In addition, the large aqueous solubility differences among benzene polycarboxylic acid isomers could be well distinguished by the proposed model. The model also has some predictive ability, and could be extrapolated to high temperatures where no experimental solubility data are available, as a preliminary estimation technique.