

544d Solubilities of Phenol and Dihydroxybenzenes in Water and Water/Ethanol Mixtures Using Monte Carlo Simulations

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A united-atom model for phenol is developed within the Transferable Potential for Phase Equilibria (TraPPE) framework to obtain an accurate description of the liquid-vapor phase equilibrium using Gibbs ensemble Monte Carlo (GEMC) simulations. Subsequently, solubilities of the several different solid polymorphs of phenol in water and water/ethanol mixtures are calculated from expanded-ensemble Monte Carlo simulations. In accordance with experiments, the most stable polymorph is found to exhibit the lowest solubility and the presence of ethanol increases the solubility significantly. Additionally, the TraPPE approach is utilized to generate potential models for the three isomers of dihydroxybenzene from phenol, and the liquid-vapor coexistence properties are obtained from GEMC simulations. Furthermore, the solubilities in water/ethanol mixture are obtained for the three different isomers.