

Temperature Dependence of Transfer Properties: Importance of Heat Capacity Effects

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Abstract

Gibbs ensemble Monte Carlo simulations were used to calculate precisely the Gibbs free energies, enthalpies, and entropies of transfer for water, 1-butanol, and *n*-octane between their own liquid phase and a helium vapor phase. It is observed that the temperature dependence of the enthalpy of transfer (i.e., the heat capacity of transfer) and not the temperature–entropy term, dominates the temperature dependence of the Gibbs free energy of transfer. Nevertheless, the curvature induced by the heat capacity in a van’t Hoff plot is small, and the van’t Hoff equation yields an enthalpy of transfer close to the value calculated directly at the mean temperature.

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