Pure Component Property Data for the IUPAC Project: Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes

R. D. Chirico[C,S], V.V. Diky, M. Frenkel
Physical and Chemical Properties Division, National Institute of Standards and Technology, Boulder, CO, U.S.A.
chirico@boulder.nist.gov

The objective of the project is to establish a database of thermodynamic properties of hydration for approximately 200 selected organic solutes at the reference conditions T = 298.15 K and p = 0.1 MPa, and as a function of temperature and pressure to the near-critical region of water. Values of hydration properties for solutes covering different molecular structures will be calculated from reliable experimental data for aqueous and pure solutes. Pure component data are required for conversion between the Gibbs energy of solution (related closely to the symmetrical limiting activity coefficient) and the Gibbs energy of hydration (related closely to the Henry's law constant). The key property for liquids and solids is the vapor pressure. In addition, a nonideality correction is, in general, also needed. Secondly, pure component data are needed for conversion between the enthalpy of solution and the enthalpy of hydration. The key property is the enthalpy of vaporization (or sublimation). In cases where the nonideality correction is needed, virial coefficients are necessary. Finally, data are required for determination of the heat capacity of hydration from the heat capacity of the aqueous solute at infinite dilution, i.e., the ideal gas heat capacity. Thirty compounds were chosen for initial evaluation. Derivation of the pure component properties for these compounds will be discussed with particular emphasis on results obtained via dynamic data evaluation with the ThermoData Engine software developed at the NIST Thermodynamics Research Center (TRC).