

Group Contribution Values at 298.15 K and 0.1 MPa for Thermodynamic Functions of Hydration of Ethers and Esters

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Group additivity methods are widely employed for reliable estimation of properties of organic compounds in different aggregate states, including properties of these compounds in aqueous solutions. In our view, the thermodynamic functions of hydration (the process of transfer of one mole of a compound from the ideal gas state to the standard aqueous solution) are the properties best suitable for a group contribution approximation. To explain this, we note that for many properties of organic compounds there are "universal" terms, independent of the composition of the organic compounds, and that these terms can be formally viewed as the properties of a compound without any groups at all. These "universal" terms appear as empirical parameters in the least-squares fit of experimental data. However, for the functions of hydration the properties of a material point (a compound without groups) are given by theory as the standard state conversion term, and can be calculated independently from the thermophysical properties of water. Various properties of aqueous solutes including: vapor-liquid distribution constants, activity coefficients at infinite dilution, Henry's constants, mutual solubility data for the case of the chemical potential, can be converted to the values of the thermodynamic functions of hydration. We discuss the necessary relations including the procedure for estimating activity coefficients of organic solutes in water that permits conversion of mutual solubility data into standard Gibbs energies of solution. Continuing our work on group contribution values for thermodynamic functions of hydration of organic compounds at 298.15 K, 0.1 MPa, we present here results for aliphatic acyclic ethers and esters.