

Bond-Contribution Method for Estimation of the Henry's Law Constant of Organic Compounds in the Extended Temperature and Pressure Range

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The EPI Suite™ (Estimation Programs Interface) is arguably the most comprehensive freeware for estimation and storage of physical/chemical property and environmental fate estimation data. A part of the suite is program HENRYWIN™ that provides the Henry's law constant at 25°C and 1 bar from experimental database, if available, and using the group contribution and the bond contribution estimation methods. The purpose of this paper is the extension of the EPI bond contribution method to thermodynamic properties that are derivatives of the Henry's law constant: partial molar volume, hydration heat capacity and hydration enthalpy. Using simple thermodynamic integration, these properties allow reliable estimation of the Henry's law constant at temperatures from 0°C to at least 100°C and at pressures from saturation to at least 10 bar. This substantially enhances accuracy of calculations based on the Henry's law constant such as environmental partitioning or various processes in remediation technologies. A newly established database of critically reviewed and thermodynamically consistent properties of hydration for selected organic solutes at reference conditions was employed as the key part of the training sets in evaluation of bond contributions for the properties of interest. Some details regarding this database will be also covered in the paper.