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Upper, Unified Physical Property Estimation Relationships

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Unified physicochemical property estimation relationships are a system of empirical and theoretical relationships that relate 20 physicochemical properties of organic molecules to each other and to chemical structure. Melting point is a key parameter in the unified physicochemical property estimation relationships scheme because it is a determinant of several other properties including vapor pressure, and solubility. This review describes the first-principals calculation of the melting points of organic compounds from structure. The calculation is based on the fact that the melting point, T_m , is equal to the ratio of the heat of melting, ΔH_m , to the entropy of melting, ΔS_m . The heat of melting is an additive constitutive property. However, the entropy of melting is not entirely group additive. It is primarily dependent on molecular geometry, including parameters that reflect the degree of restriction of molecular motion in the crystal to that of the liquid.

Symmetry, eccentricity, chirality, flexibility and hydrogen bonding each affect molecular freedom in different ways and thus make different contributions to the total entropy of fusion. The relationships of these entropy-determining parameters to chemical structure are used to develop a reasonably accurate means of predicting the melting points of over 2000 compounds.

Biography:

Samuel Yalkowsky received his Ph.D. in pharmaceutical chemistry from the University of Michigan in 1969. He worked at The Upjohn Company from 1969 until 1982 when he joined the faculty of the University of Arizona. His work has led to over 280 scientific publications and patents and six books. His early work dealt with the alteration of solubility and the formulations of insoluble drugs. The formulation work includes the development of novel dosage forms and the pharmaceutical evaluation of parenteral formulations. His current interest is the relationship between physicochemical properties and chemical structures.