Prediction of the Vapor Pressure of Non-Electrolyte Organic Compounds *via* Group Contributions and Group Interactions

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A new group contribution method for the estimation of vapor pressure data has been developed. The method is based on the structural group definitions with minor modifications of a recently published method for the normal boiling point by Nannoolal et al. [1]. The model was extended to allow the prediction of vapor pressure data with special attention to the low pressure region. In case of available experimental information, the vapor pressure equation can be adjusted in order to reproduce vapor pressure data with high accuracy. Though not temperature explicit, this correlation equation converges very fast and secure in case of boiling point calculations at given pressure. For the vapor pressure prediction, only the molecular structure of the compound and a fixed point, usually the normal boiling point, are used, and the method estimates the slope of the change in logarithm vapor pressure and reciprocal temperature. The results of the new method are compared to several currently-used correlative models, for e.g. the Antoine equation, and have proven to have a similar accuracy. Moreover, the structural groups contain information about the chemical nature of a compound and, thus, can be proven to be more reliable than the correlative models. Structural groups were defined in a standardized form and fragmentation of the molecular structures was performed by an automatic procedure to eliminate any arbitrary assumptions.

[1] Y. Nannoolal, J. Rarey, D. Ramjugernath, W. Cordes, *Fluid Phase Equilib.* **226,** 45-63, (2004).