Prediction of Critical Properties of Non-Electrolyte Organic Compounds via Group Contributions and Group Interactions

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A new group contribution method for the estimation of critical property 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 performance of the proposed models has been compared with 10 well known estimation methods from literature and the results indicate that the new model is significantly more reliable and the range of applicability is larger. In addition, the new models have been carefully constructed to prevent unrealistic extrapolations. The critical property data set used in this work after extensive data evaluation, consisted of 588 critical temperatures, 486 critical pressures and 348 critical volumes from the Dortmund Data Bank (DDB). 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).