

Densities and Isothermal Compressibilities of Ionic Liquids - Data Retrieval, Modelling and Application

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Ionic liquids are frequently suggested as potential replacements of volatile organic solvents currently used in industry. However, presently only limited physical property data are available for engineers to use when designing new processes or retrofitting old systems. There have been a number of papers in the recent years describing methods for the correlation and prediction of volumetric properties of ionic liquids, such as by Ye/Shreeve [1], Gardas/Coutinho [2] and Jacquemin et al. [3], among others. This suggests a widespread interest in methods for obtaining volumetric properties of ionic liquids. This paper describes the use of a two-parameter, corresponding-states form for direct correlation function integrals in liquids to represent the volumetric properties of ionic liquids over wide ranges of temperature and pressure adapted from the method of Campanella et al. [4] which is an isothermal equation of state. Molecular parameters (V^* and T^*) for more than 30 different ionic liquid systems have been obtained by reduction of PVT data. The results show excellent agreement with the experimental data for all of the substances over all data ranges of condition. Establishing group contributions for these parameters has also been explored. An appealing aspect of this correlation is that it can be integrated with predictions of gas solubilities in liquids and liquid mixtures for reduced densities from 1.5 to more than 3.65, as shown by Campanella et al. [4]. Examples of this application are also given here. Finally, we have explored fitting of the data using the three-parameter, corresponding-states form for direct correlation function integrals by Huang and O'Connell [5]. That method gives even better results.

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