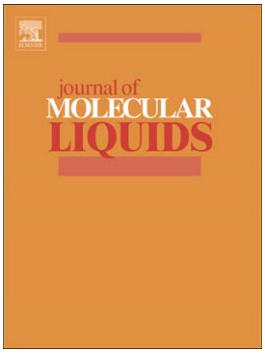

On the evaluation of density of ionic liquid binary mixtures: Modeling and data assessment

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On the Evaluation of Density of Ionic Liquid Binary Mixtures: Modeling and Data Assessment

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Abstract: The unique and exciting properties of ionic liquids (ILs) have driven much interest in using them in many industrial applications. The thermophysical properties of pure ILs and their binary mixtures with water or alcohols are required for various usages. In this communication, in order to determine the density values of ILs, a large data bank containing a large number of ILs binary mixture (1510 data sets) was gathered from previously published literature. The Least Square Support Vector Machine (LSSVM) strategy as a reliable and powerful computational prediction method was utilized for predicting the density of binary mixtures at atmospheric pressure. Additionally, a second LSSVM model was developed for predicting the density of 1-butyl-3-methylimidazolium tetrafluoroborate + methanol binary mixture at different pressures using 405 data points. Coupled Simulated Annealing (CSA) optimization tool was employed in order to optimize the parameters of both models. For the first model, the inputs were density of each compound at standard condition, temperature, and mole fraction of IL and for the second model temperature, pressure, and mole fraction of IL were considered as the input parameters. Moreover, in order to evaluate the performance of these models, various graphical and statistical error analyses were performed. These analyses demonstrated that the developed models are able to predict the density of ILs with high accuracy and reliability. Finally, in order to detect the applicability domain of the models, the Leverage approach was applied, which led to detection of the probable data outliers. According to this approach, the entire experimental data sets in both models seem to be reliable except six data points in each model.

Keyword: Ionic liquid; Density; Binary mixtures; Support vector machine; Leverage approach.

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