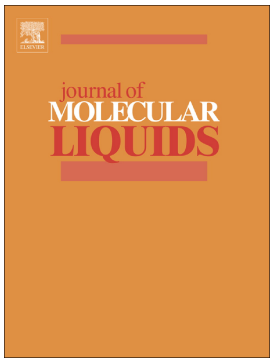

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PII: S0167-7322(16)33941-1
DOI: doi: 10.1016/j.molliq.2017.02.034
Reference: MOLLIQ 6947

To appear in: *Journal of Molecular Liquids*

Received date: 7 December 2016
Revised date: 10 February 2017
Accepted date: 11 February 2017

Please cite this article as: Ali Barati-Harooni, Adel Najafi-Marghmaleki, Milad Arabloo, Amir H Mohammadi , Chemical structural models for prediction of heat capacities of ionic liquids. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi: 10.1016/j.molliq.2017.02.034

Chemical Structural Models for Prediction of Heat Capacities of Ionic Liquids

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Abstract - Heat capacity of ionic liquids (ILs) is an important property which is needed in various scientific and engineering problems. Hence, it is required to develop accurate and general models for prediction of this property in various conditions from both academic and industrial perspectives. This work highlights the application of three models namely Least Square Support Vector Machine optimized by Coupled Simulated Annealing optimization algorithm (CSA-LSSVM), Gene Expression Programming (GEP) and Adaptive-Neuro Fuzzy Inference System optimized by Hybrid method (Hybrid-ANFIS) for prediction of heat capacity of ILs. The input parameters of the models are temperature, molecular weight of IL, number of carbon atoms in cation part of IL (C_C), number of carbon atoms in anion part of IL (C_A), number of IL nitrogen atoms (*N*), number of IL sulfur atoms (*S*), number of IL oxygen atoms (*O*), number of IL phosphorous atoms (*P*), number of IL fluorine atoms (*F*), number of IL bromine atoms (*Br*), number of IL chlorine atoms (*Cl*), number of IL boron atoms (*B*) and the number of hydrogen atoms in anion part (nH_A). An extensive data set including 2940 data points from 56 ILs was used to implement the models. Predictions of developed models were evaluated by statistical and graphical validation approaches. Moreover, comparison was also made between outcomes of developed models and predictions of recently developed literature correlations. Results showe that the models are accurate and reliable. However, the predictions of CSA-LSSVM model were better than GEP and Hybrid-ANFIS models. In addition, the developed models outperform the literature correlations for prediction of heat capacity of ILs.

Keywords - Ionic liquid (IL); Heat capacity; Model; Prediction; Chemical structure.

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