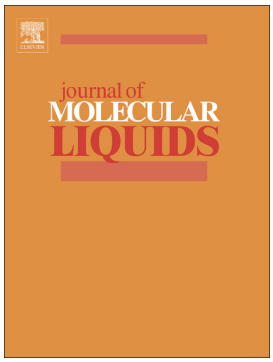

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Novel molecular descriptors for prediction of H_2S solubility in ionic liquids

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Abstract: Molecular descriptors are very important input parameters for establishing properties prediction models of materials, such as ionic liquids (ILs). In this work, as a new class of molecular descriptors, namely, electrostatic potential surface (S_{EP}) is proposed to predict one of the important representative properties of ILs, i.e. the H_2S solubility in ILs. 1318 experimental data points of 28 ILs, including 7 cations and 12 anions covering diverse temperatures and pressures, have been gathered from 15 references. According to the qualitative analyses, it is found that anions play a more important role than cations for the H_2S solubility in ILs, besides the anions with stronger hydrogen-bond basicity have higher capacities to absorb H_2S. Combining the S_{EP} descriptors with the extreme learning machine (ELM) algorithm, two new

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