

عنوان مقاله:

A novel SVM-GCM model for prediction of surface tension of some ionic liquids at different temperatures

محل انتشار:

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خلاصه مقاله:

In this study, a novel group contribution method (GCM) is developed to predict the surface tension of ionic liquids (ILs) using support vector machine (SVM) algorithms. A data set including 1225 experimental data for 133 ionic liquids collected from various references is used to develop and assess the predictive capability of the model. The data set covers a temperature range of 278.15 through 470.56 K and a surface tension range of 19.15 through 70.30 mN.m-1. It employs a total of 45 anion-cation groups plus temperature to predict the surface tension. To better distinct the effects of anion and cation on the surface tension of ionic liquids, 5 cation groups, 36 anion groups and 4 substituted functional groups attached to the cation group, were implemented. The results of this method show an average .absolute relative deviation (AARD) of 3.48% from experimental data

کلمات کلیدی:

Surface tension, Ionic liquids, Group contribution method, Support vector machine

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