

عنوان مقاله:

Prediction of viscosity of ionic liquids by using of new coupling of group contribution method and support vector machine (GCM-SVM) at different temperatures and pressures

محل انتشار:

کنفرانس بین المللی مهندسی و علوم کاربردی (سال: 1394)

تعداد صفحات اصل مقاله: 21

نویسنده:

Hoda Keshtkar - Department of Chemistry ,Shahrood University of Technology , Shahrood , Iran

خلاصه مقاله:

In this work, the viscosity of ionic liquids at different temperatures and pressures was estimated with a simple group contribution method. The proposed method was applied using a support vector machine algorithms. A total data set of 2735 experimental viscosity data points under a wide range of temperature and pressure for 273 ionic liquids (ILs), is employed to train and verify the model. Experimental data of 218 ionic liquids (2282 data points) with viscosity in a range of 1.7 to 21829 (cP) at temperatures in a range of 253.15 K to 500 K and pressures in a range of 0.1 MPa to 300 MPa were used to obtain the contributions for the cation–anion groups in a correlation set . Then, the viscosities of another 55 ionic liquids (453 data points) were predicted, and the results were compared with experimental data available in the literature. The results show that this group contribution method represents an excellent alternative for the estimation of the viscosity of diverse ionic liquids at different temperatures and pressure from the knowledge of their molecular structure with an average deviation of 4.411% and a correlation coefficient of 0.9697.

کلمات کلیدی:

Viscosity, Ionic liquids, Group contribution method, Support vector machine

لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/483285>

