عنوان مقاله:

QSPR Models of Physicochemical Properties ofAlkyl Benzenes derivatives by Topological Indices based on MLR method

محل انتشار:

اولین کنفرانس ملی آنالیز داده ها (سال: 1402)

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خلاصه مقاله:

Quantitative Structure–Activity Relationship (QSAR) / Quantitative Structure – Property Relationship (QSPR) model have been used to the prediction biological activity or physico-chemical property. Physicochemical properties of alkylbenzenes can be applied to separate pure ingredient from alkylbenzenes mixture. In this study multiple linear regression (MLR) method, integrated with topological indices was used to the prediction thermal energy (Eth), heat capacity in constant volume (Cv) and entropy (S) of ۵۸ alkylbenzenes. Topological indices such as Wiener(W) index, Hyper Wiener(WW) Index, Wiener polarity(Wp) Index, Harary(H) Index, Balaban (J)index, and Randic(۱X) index are calculated for analysis. The obtained models were validated using leave-one-out (LOO) cross-validation; internal datasets. The squares of correlation coefficients (R۲) for MLR models of Eth, Cv and S were calculated to be ۰.۹۲۳, ۰.۸۱۵ and ۰.۶۶۴ respectively. Results showed that the predictive ability of the models was satisfactory, and these models can be used to predict the mentioned properties of similar alkyl benzenes.

کلمات کلیدی:

Topological Indices, alkyl benzenes; Quantitative Structure-Property Relationship Study; Multivariate Linear Regression

لینک ثابت مقاله در پایگاه سیویلیکا: