عنوان مقاله:

Determining the octanol-water partition coefficient of amines using MLR method

نویسندگان:

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خلاصه مقاله:

In this study, the MLR method based on QSPR method was applied to predict the LogP of 31 differenttype amines. The results of experimental for used molecules were compared with the results of MLR calculations andwas represented that minimum Z Length, minimum projection area, Maximum Z Length indices are the best descriptorsfor predicting the values of LogP of used amines. The best model in this study indicated that those structuraldescriptors, play an important role in effect on LogP of amines. For the first time, the relationship between LogP ofamines and some molecular indices using SPSS and multiple linear regression model is investigated. The obtainedresults demonstrated that there are good relationships between some geometrical indices of this class amines.

کلمات کلیدی:

Amines , Octanol-Water Partition Coefficient , Molecular Descriptors

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