Critical Pressure Prediction QSPR Model for Organic Compounds Including Oxygen, Sulfur, and Nitrogen

오지예, 양대륙†, 박기호, 김양수[1], 박태윤[1], 진윤태
고려대학교; [1](주)켐에쎈
(dryang@korea.ac.kr†)

It is very difficult to determine various physical properties of chemicals through experiments because of the cost and the risk of handling hazardous substances. A reliable prediction of physicochemical property can be an alternative instead of experiments. In this research, we predicted critical pressure of organic compounds with QSPR model. The model shows high prediction performance and it stems from big number of organic samples to create the model, quantum mechanical calculation for 3D structure optimization, and proper descriptor selection algorithm. The best prediction performance for hydrocarbon group is 0.861 bar in average absolute error and that for nonhydrocarbon organic compounds group is 1.87 bar in average absolute error.