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

오지예, 양대륙[1,†], 김양수[2], 박태윤[2]
고려대학교; [1]고려대학교 화공생명공학과; [2](주)켐에쎈
(dryang@korea.ac.kr[†])

Critical pressure is one of the most important chemical properties. Prediction of critical pressure can help reduce the effort to repeat experiments and collect data. Critical pressures of diverse organic chemicals were estimated by QSPR model. QSPR model was constructed with forward selection, genetic algorithm, multi linear regression and neural network. Forward selection and genetic algorithm were used for the purpose of selecting appropriate descriptors which can explain critical pressure efficiently. Multi linear regression and neural network figured out linear and non-linear mathematical relationship between selected descriptors and critical pressure respectively. These procedures were applied to hydrocarbon group and nonhydrocarbon organic compound group independently. Nonhydrocarbon organic compound group contains organic compounds like oxygen, nitrogen and sulfur. The results of prediction are quite satisfying in that average absolute errors of hydrocarbon and nonhydrocarbon group is 0.9bar and 0.6bar respectively.