Prediction of Critical Pressure of not only Pure Organic Compounds but also Organic Compounds with Halogen, N, S, P and Si using QSPR

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Misinformation about critical pressure can cause severe industrial disasters. In this reason, chemical engineers try to find the exact critical pressure of chemicals through experiments but these works require highly expensive cost. Prediction of critical pressure reduces experimental cost significantly by proposing the starting point of critical pressure experiments. In this research, critical pressure is estimated using quantitative structure-property relationship (QSPR). The coverage of the research contains not only pure organic compounds but also organic chemicals with halogen, nitrogen, sulfur, phosphorus and silicon. Many descriptors, 1978 descriptors, are used to estimate and the relationship between critical pressure and selected descriptors is analyzed. Performance of prediction in terms of coefficient of determination (R^2) is 0.99 and 0.96 each for pure organic compounds group and the other group with halgoen, N, S, P and Si.