

عنوان مقاله:

Prediction of boiling point and water solubility of crude oil hydrocarbons using sub-structural molecular fragments method

محل انتشار:

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خلاصه مقاله:

The quantitative structure–property relationship (QSPR) method is used to develop the correlation between structures of crude oil hydrocarbons (80 compounds) and their boiling point and water solubility. Sub-structural molecular fragments (SMF) calculated from structure alone were used to represent molecular structures. A subset of the calculated fragments selected using stepwise regression (forward and backward steps) (SR) was used in the QSPR model development. Multiple linear regressions (MLR) are utilized to construct the linear prediction model. The prediction results agrees well with the experimental values of these properties. The comparison results indicate the superiority of the presented models and reveal that it can be effectively used to predict the boiling point temperatures and water solubility values of crude oil hydrocarbons from the molecular structures alone. The stability and predictivity of the proposed models were validated using internal validation (leave one out and leave many out) and external validation. Application of the developed models to test set of 16 compounds demonstrates that the new models are .reliable with good predictive accuracy and simple formulation

کلمات کلیدی:

Boiling point, water solubility, crude oil hydrocarbon, ISIDA-QSPR, prediction

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