

O8 : Electrochemical determination of logP of ferrocene derivatives

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Abstract:

We present in this work the experimental determination of octanol/water partition coefficients of ten selected ferrocene derivatives using electrochemical and spectrophotometrical techniques, the first is based on square wave voltammetry and the second is based on the adsorption of UV-vis. We have investigated the accuracy of obtained experimental partition coefficients values of logP for all studied ferrocene derivatives with those obtained by calculation using the known atom-additive method. It was shown that experimental partition coefficients are in good agreement with calculated values. The average absolute error of log P is 0.11, and the average relative error is 23 %.

Key word: experimental logP , theoretical partition coefficient, substituted ferrocene, lipophilicity, QSAR.