

PREDICTION OF OCTANOL-WATER PARTITION COEFFICIENTS

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ABSTRACT

The partitioning of pollutants is traditionally expressed in environmental science with the octanol-water (K_{ow}) coefficient, which is related to the bioconcentration factor i.e. the accumulation of a pollutant in the lipid phase of an aquatic organism. In this work, K_{ow} calculations are reported for a number of pollutants with two thermodynamic models, the UNIFAC by Chen et al., and the novel equation of state abbreviated as sCPA developed by IGVP Ltd. Very satisfactory K_{ow} results are obtained with the sCPA which are generally closer to the experimental values compared to the classical UNIFAC method.