

Octanol-water partition coefficients of ionic liquids

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Room-temperature ionic liquids (ILs) are attracting growing interest as alternative reaction media for catalytic transformations, which are non-volatile, thermally stable and highly polar. However, few published data are available for their environmental behavior and ecological effects. In toxicology, octanol/water partition coefficient which is considered to model blood/lipid partition is critical to understand the tendency of a chemical to cross biological membranes. In this study, octanol/water partition coefficients of 1-butyl-3-methylimidazolium ILs containing hexafluorophosphate ($[\text{PF}_6]^-$) and bistrifluoromethane-sulfonimide ($[\text{Tf}_2\text{N}]^-$) were investigated. The experimental partition coefficient values of ILs increased with increasing the initial concentration of ILs. These results were understood by the partition model of ILs. With decreasing and increasing the concentration of ILs, the experimental partition coefficient values converge to the partition coefficients of cation and ion pair of ILs. The partition coefficients and dissociation constants of ILs were determined with this partition model.