n-Alcohol/Water Partition Coefficients for Decachlorobiphenyl (PCB 209)

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Measurements of n-octanol/water partition coefficients (K_{ow}) for highly hydrophobic chemicals are extremely difficult and are rarely made, in part due to the large volumes of water typically needed to quantify these compounds in the aqueous phase. An extrapolation approach using the partition coefficients for shorter-chain, more water-soluble n-alcohols is being evaluated. The increased water solubility of these alcohols is predicted to increase the amount of chemical in the water phase at equilibrium, thus lowering the partition coefficient. Theoretically, the successive partition coefficients between water and n-butanol, n-pentanol, n-hexanol, and n-heptanol could be extrapolated back to estimate n-octanol/water. As a proof of principle, the partition coefficients of PCB 209 in these n-alcohol/water systems are being measured using the OECD 123 Slow Stir method to evaluate this approach. If successful with PCB 209, the approach will be later applied to more hydrophobic chemicals (e.g., brominated flame retardants).

Our initial log n-butanol/water partition coefficients measured for PCB 209 were 5.19 ± 0.04, showing a significant depression from the log K_{ow} of 8.22. Partition coefficients for PCB 209 in n-pentanol, n-hexanol, n-heptanol, and n-octanol will be provided and discussed.

This abstract does not necessarily reflect U.S. EPA policy

Key words: K_{ow}, decachlorobiphenyl, Slow Stir, Hydrophobic chemicals

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