Accepted Manuscript

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PII: S0045-6535(17)31914-8

DOI: 10.1016/j.chemosphere.2017.11.137

Reference: CHEM 20334

To appear in: *ECSN*

Received Date: 5 October 2017

Revised Date: 21 November 2017

Accepted Date: 22 November 2017

Please cite this article as: Tebes-Stevens, C., Patel, J.M., Koopmans, M., Olmstead, J., Hilal, S.H., Pope, N., Weber, E.J., Wolfe, K., Demonstration of a consensus approach for the calculation of physicochemical properties required for environmental fate assessments, *Chemosphere* (2017), doi: 10.1016/j.chemosphere.2017.11.137.

Demonstration of a consensus approach for the calculation of physicochemical properties required for environmental fate assessments

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Abstract

Eight software applications are compared for their performance in estimating the octanol-water partition coefficient (K_{ow}), melting point, vapor pressure and water solubility for a dataset of polychlorinated biphenyls, polybrominated diphenyl ethers, polychlorinated dibenzodioxins, and polycyclic aromatic hydrocarbons. The predicted property values are compared against a curated dataset of measured property values compiled from the scientific literature with careful consideration