

Accepted Manuscript

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

Caroline Tebes-Stevens, Jay M. Patel, Michaela Koopmans, John Olmstead, Said H. Hilal, Nick Pope, Eric J. Weber, Kurt Wolfe



PII: S0045-6535(17)31914-8

DOI: [10.1016/j.chemosphere.2017.11.137](https://doi.org/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.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

3
4 Caroline Tebes-Stevens^{†*}, Jay M. Patel[‡], Michaela Koopmans[§], John Olmstead[§], Said H. Hilal[†], Nick
5 Pope[¥], Eric J. Weber[†], and Kurt Wolfe[†]

6 [†] U.S. Environmental Protection Agency, National Exposure Research Laboratory, Athens, Georgia
7 30605, United States

8 [‡] ORISE Fellow, U.S. Environmental Protection Agency, National Exposure Research Laboratory, Athens,
9 Georgia 30605, United States

10 [§] ORAU, U.S. Environmental Protection Agency, National Exposure Research Laboratory, Athens,
11 Georgia 30605, United States

12 [¥] Independent Contractor, Tifton, Georgia

13 Corresponding Author

14 * Phone: (706) 355-8218; e-mail: stevens.caroline@epa.gov

15
16 **Abstract**

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

Download English Version:

<https://daneshyari.com/en/article/8852379>

Download Persian Version:

<https://daneshyari.com/article/8852379>

[Daneshyari.com](https://daneshyari.com)