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QSAR Prediction Reporting Format (QPRF) for the Henry's Law Constant of Phthalic Anhydride (CAS or 85-44-9)

Summary

The Henry's law constant (HLC) of phthalic anhydride was predicted using the Estimation Program Interface EPI-Suite version 4.11.

The HLC was estimated to be

Bond estimation method: HLC = 6.43×10^{-1} Pa m³/mol HLC = 6.35×10^{-6} atm m³/mol HLC = 2.59×10^{-4}



The bond method was chosen for this estimation instead of the group method because an independent evaluation of Altschuh et al. (1999) for a diverse set of organic chemicals found the bond method more accurate than the group method.

1. SUBSTANCE:

- **1.1** Chemical name: phthalic anhydride
- **1.2 CAS number:** 85-44-9
- **1.3 EC number**: 201-607-5
- **1.4** Structural formula



- **1.5 Empirical formula:** C8H4O3
- **1.6 Structure codes:**
 - **a. SMILES:** O=C1OC(=O)c2cccc12
 - **b.** InChI: InChI=1/C8H4O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-4H
 - c. Other structural representation: None.
 - d. Stereo chemical features: Not applicable.
- **1.7 Molecular weight:** 148.12 g/mol

2. GENERAL INFORMATION

- **2.1 Date of QPRF:** 2017-05-02
- 2.2 **QPRF author and contact details:** Dr. Alexandra Heilkenbrinker, Currenta GmbH & Co. OHG, Department Analytics/ Product Safety / Ecotoxicology; CHEMPARK Leverkusen, Building Q18, 51368 Leverkusen (Germany)

3. PREDICTION

- **3.1** Endpoint (OECD Principle 1)
 - a. Endpoint: Henry's Law Constant (HLC)
 - b. Dependent variable:

Henry's Law Constant (HLC)

- **3.2** Algorithm (OECD Principle 2)
 - a. Model or sub model name:

Individual model HENRYWIN included in the Estimation Programs Interface (EPI) Suite.



b. Model version:

HENRYWIN v3.20 included in EPI-Suite v4.11, 2000-2012.

c. Reference to QMRF:

"Henry's Law Constant QSAR Model Reporting Format" Currenta, 2011-09-14

d. Predicted value (model result):

Bond estimation $HLC = 6.43 \times 10^{-1} \text{ Pa m}^3/\text{mol}$ $HLC = 6.35 \times 10^{-6} \text{ atm m}^3/\text{mol}$ $HLC = 2.59 \times 10^{-4}$

e. Predicted value (comments):

No information available.

f. Input for prediction:

A CAS number was entered in the initial data entry screen. In the structure window, the molecular weight, structural formula and the structure of the input SMILES notation is shown.

g. Descriptor values:

For phthalic anhydride the following fragment descriptors were applied: bond estimation method

class	bond contribution description	value
Hydrogen	4 Hydrogen to Carbon (aromatic) Bonds	-0.6172
Fragment	6 Car-Car	1.5828
Fragment	2 Car-CO	2.4775
Fragment	2 CO-O	0.1429

3.3 Applicability domain (OECD principle 3)

a. Domains:

i. Molecular weight:

With a molecular weight of 148.12 g/mol the substance is within the range of the training set (26.04 - 451.47 g/mol).

ii. Structural fragment domain:

Regarding the structure, the fragment descriptors used by the program for the estimation are complete and listed in Appendix D, E of the HENRYWIN help file.

- iii. Mechanism domain: No information available.
- iv. Metabolic domain, if relevant: Not relevant.

v. further limitation:

The calculated value reflects the properties of the unhydrolyzed molecule without taking into account the sensitivity of phthalic anhydride towards hydrolysis

b. Structural analogues: No information available.



c. Considerations on structural analogues: No information available.

3.4 The uncertainty of the prediction (OECD principle 4)

Phthalic acid is not highly complex and the rules applied for the substance appears appropriate. An individual uncertainty for the investigated substance is not available.

3.5 The chemical and biological mechanisms according to the model underpinning the predicted result (OECD principle 5).

No information available.

4. ADEQUACY (OPTIONAL)

4.1 Regulatory purpose:

The data may be used under any regulatory purpose.

4.2 Approach for regulatory interpretation of the model result:

If no experimental data are available, the estimated value may be used to fill data gaps needed for hazard and risk assessment. Further the value is used for other calculations.

4.3 Outcome:

The prediction of the Henry's Law Constant yields a useful result for further evaluation.

4.4 Conclusion:

The result is considered as useful for regulatory purposes. The calculated value reflects the properties of the unhydrolyzed molecule without taking into account the sensitivity of phthalic anhydride towards hydrolysis.

A. Hilbubrinho

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