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QSAR Prediction Reporting Format (QPRF)

for the log Koc estimation of Phthalic anhydride

(CAS no. 85-44-9)

Summary

The organic carbon partition coefficient log Koc of phthalic anhydride was estimated using the Estimation Program Interface EPI-Suite version 4.11 (KOCWIN) and calculated as:

a) MCI method : log Koc = 1.00, Koc = 10.00 L/kg

b) Log Kow method : log Koc = 1.35, Koc = 22.47 L/kg

For estimation of log Koc according to log Kow method an experimentally determined log Kow of 1.60 was used (experimental DB: http://esc.syrres.com/interkow/EpiSuiteData.htm).

1 SUBSTANCE

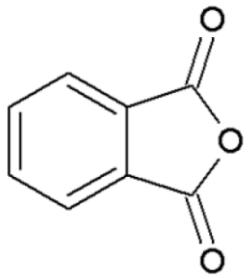
1.1 Chemical name: phthalic anhydride

1.2 CAS number: 85-44-9

1.3 EC number: 201-607-5

1.4 EC name: phthalic anhydride

1.5 Structural formula:



1.6 Empirical formula: $C_8H_4O_3$

1.7 Structure codes:

a) SMILES: O=C1OC(=O)c2ccccc12

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) Stereochemical features: none

1.8 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, Building Q18, 51368 Leverkusen (Germany).

3 PREDICTION

3.1 Endpoint (OECD Principle 1)

a) Endpoint: Organic carbon partition coefficient, given as log Koc.

b) Dependent variable: KOCWIN estimates log Koc with two separate estimation methodologies:

(1) Estimation using first-order Molecular Connectivity Index (MCI) and

(2) Estimation using log Kow (octanol-water partition coefficient).

3.2 Algorithm (OECD Principle 2)

a) Model or submodel name: Individual model KOCWIN included in the Estimation Programs Interface (EPI) Suite.

b) Model version: KOCWIN v2.00 included in EPISuite v 4.11, 2000-2012.

c) Reference to QMRF: QMRF of Currenta GmbH & Co. OHG, 19 May 2011

d) Predicted value (model result):

a) MCI method: log Koc = 1.00, Koc = 10.00 L/kg

b) Log Kow method: log Koc = 1.35, Koc = 22.47 L/kg

e) Predicted value (comments):

Log Koc according to MCI method is calculated using the formula:

log Koc = 0.5213 MCI + 0.60 + ΣPfN

(ΣPfN is the sum of all relevant correction factor coefficients multiplied by the number (N) of that factor in each chemical structure)

Log Koc according to the log Kow method is calculated using the formula (depending on the polarity of the substance):

log Koc = 0.55313 log Kow + 0.9251 + ΣPfN (polar substances)

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:

Log Kow method:

For estimation of log Koc according to log Kow method an experimentally determined log Kow of 1.60 was used (experimental DB: http://esc.syrres.com/interkow/EpiSuiteData.htm) and the following fragment descriptors were applied:

Type	No. of Fragments	Fragment	Fragment Description
Fragment Correction	1	2	Misc (C=O) Group (aliphatic attach)

MCI method: For log Koc estimation of phthalic anhydride according to MCI method the following fragment descriptors were applied:

Type	No. of Fragments	Fragment	Fragment Description
Fragment Correction	1	2	Misc (C=O) Group (aliphatic attach)

3.3 Applicability domain (OECD principle 3)

a) Domains:

i. Molecular weights:
With a molecular weight of 148.12 g/mol the substance is within the range of the training set (32 - 665 g/mol) as well as in the range of the validation set (27 991 g/mol).

ii. Structural fragment domain:
Regarding the structure of phthalic anhydride the fragment descriptors found by the program are complete and listed in Appendix D (KOCWIN Fragment and Correction Factor descriptors).

iii. Mechanism domain:
No information available.

iv. Metabolic domain, if relevant:
Not relevant.

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 anhydride is not highly complex and the rules applied for the substance appear 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, classification and labelling and PBT / vPvB assessment. Further the value is used for other calculations.

4.3 Outcome:

The prediction of organic carbon partition coefficient 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

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(Product Safety / Ecotoxicology)