CURRENTA

LANXESS Deutschland GmbH
Kennedyplatz 1
50569 Köln
Germany

Analytics
Product Safety / Ecotoxicology
Dr. Alexandra Heilkenbrinker
Currenta GmbH & Co. OHG
CHEMPARK
51368 Leverkusen
Germany

Phone: +49 214-30-48379
alexandra.heilkenbrinker @currenta.de

Registered office: Leverkusen
Registered:
Local Court of Cologne
HR A 20833

A company of
Bayer and LANXESS

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QSAR Prediction Reporting Format (QPRF) for the log Kow estimation of Phthalic Anhydride (CAS no. 85-44-9)

Summary

The octanol-water partition coefficient (log Kow) of phthalic anhydride was predicted using the Estimation Program Interface (EPI) Suite version 4.11.

The **log Kow** was estimated to be: **2.0688**.

1. SUBSTANCE

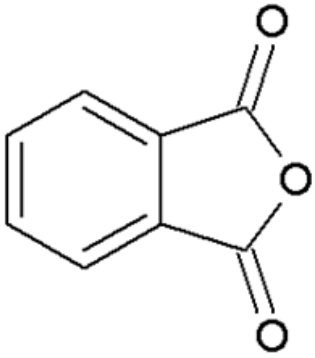
1.1 Chemical name: phthalic anhydride

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:** not applicable

1.8 Molecular weight: 148.12 g/mol

2. GENERAL INFORMATION

2.1 Date of QPRF: 2016-12-16.

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:

Logarithmic octanol-water partition coefficient (log Kow)

b. Dependent variable:

log Pow *or* log Kow

3.2 Algorithm (OECD Principle 2)

a. Model or submodel name:

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

b. Model version:

KOWWIN v1.68 included in EPI Suite v4.11, ©2000 - 2012

c. Reference to QMRF:

"QSAR Model Reporting Format (QMRF) for log Kow estimation", Currenta GmbH & Co. OHG, 2011-05-19.

d. Predicted value (model result):

log Kow = 2.0688

e. Predicted value (comments):

No information available.

f. Input for prediction:

A SMILES notation 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:

The molecule is separated into distinct atom/fragments using an Atom/Fragment Contribution method. Based on structure of the molecule, various steric interactions, hydrogen-bondings, and effects from polar functional substructures were identified and individual correction factors were selected through a tedious process of correlating the differences (between log Kow estimates from atom/fragments alone and measured log Kow values) with common substructures.

For phthalic anhydride the following fragment descriptors were applied:

Type	NUM	Fragment	Fragment Description
Fragment	6		Aromatic Carbon
Fragment	2	-C(=O)O-	[ester, aromatic attach]
Factor	2		Cyclic ester [di-carbonyl type] correction

3.3 Applicability domain (OECD principle 3)

a. Domains:

i. Molecular weights:

With a molecular weight of 148.12 g/mol phthalic anhydride is within the range of the training set (18.02 - 719.92 g/mol) as well as in the range of the validation set (27.03 - 991.15 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 (KOWWIN Fragment and Correction Factor descriptors). Additionally phthalic anhydride is not listed in Appendix F (Compounds that exceed the Fragment & Molecular Weight Domains).

iii. Mechanism domain: No information available

iv. Metabolic domain, if relevant: Not relevant.

b. Structural analogues: Optional

c. Considerations on structural analogues: Optional

3.4 The uncertainty of the prediction (OECD principle 4)

Phthalic anhydride is not highly complex and the applied rules 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 is used to fill data gaps needed for hazard and risk assessment, classification and labelling and PBT / vPvB assessment. Further the value can be used for other calculations.

4.3 Outcome:

The prediction of the logarithmic octanol-water partition coefficient yields a useful result for further evaluation.

4.4 Conclusion:

The result is considered as useful for regulatory purposes.

Dr. Alexandra Heilkenbrinker
(Product Safety / Ecotoxicology)