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QSAR Prediction Reporting Format (QPRF) for the vapour pressure estimation of bis(2-ethylhexyl) tetrabromophthalate (CAS No. 26040-51-7)

Summary

The vapour pressure (Vp) of bis(2-ethylhexyl) tetrabromophthalate was predicted using the Estimation Program Interface (EPI) Suite version 4.11.
The following parameters were taken for calculation:

- Boiling point: 539.75°C (calculated by MPBPWIN v1.43)

Using the modified Grain method, the vapour pressure was estimated to be:

$3.56*10^{-7}$ Pa at 25°C

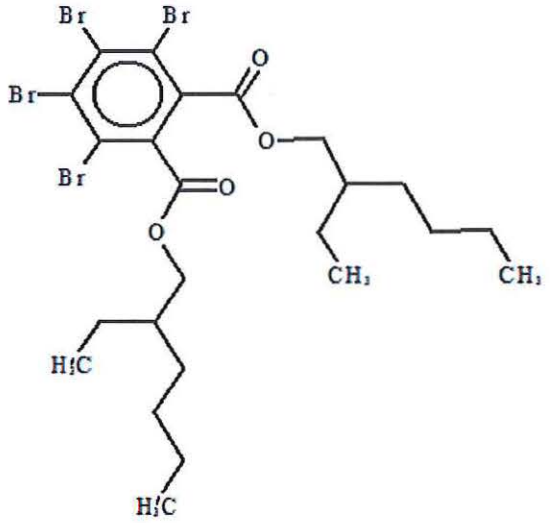
1. SUBSTANCE:

1.1 Chemical name: bis(2-ethylhexyl) tetrabromophthalate

1.2 CAS number: 26040-51-7

1.3 EC number: 247-426-5

1.4 Structural formula:



1.5 Empirical formula: $C_{24}H_{34}Br_4O_4$

1.6 Structure codes:

a. **SMILES:**
O=C(OCC(CCCC)CC)c(c(c(c(c1Br)Br)Br)C(=O)OCC(CCCC)CC)c1Br

b. **InChI:** Not available.

c. **Other structural representation:** None.

d. **Stereo chemical features:** Not applicable.

1.7 Molecular weight: 706.15 g/mole

2. GENERAL INFORMATION

2.1 Date of QPRF: 2013-03-06

2.2 QPRF author and contact details: Currenta GmbH & Co. OHG, CHEMPARK, Building Q18, 51368 Leverkusen (Germany)

3. PREDICTION

3.1 Endpoint (OECD Principle 1)

a. **Endpoint:**
Vapour pressure

b. **Dependent variable:**
Vapour pressure

3.2 Algorithm (OECD Principle 2)

a. Model or sub model name:

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

b. Model version:

MPBPWIN v1.43 included in EPI-Suite v4.11, 2000 - 2012

c. Reference to QMRF:

QMRF Currenta, 2011-08-08

d. Predicted value (model result):

Vapour pressure: $3.56*10^{-7}$ Pa at 25°C

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. If available, experimentally determined values of melting point and boiling point are taken for input.

g. Descriptor values:

As bis(2-ethylhexyl) tetrabromophthalate is a liquid, the model uses only the boiling point for estimation.

The boiling point was experimentally determined to be > 300°C at 1013 hPa (BTS, 2012). This value was not used for the calculation of the vapour pressure as this would lead to an unrealistic result and the vapour pressure would be overestimated to a large extent. As a conclusion the boiling point was calculated instead.

The following parameters were applied:

Boiling point: 539.75°C at 1013 hPa (calculated by MPBPWIN v1.43)

Ref.: BTS, 2012: "Study Report, Standard information requirements and classification (REACH & CLP) for bis(2-ethylhexyl) tetrabromophthalate (Uniplex FRP45), CAS-No: 26040-51-7" Bayer Technology Services, Chempark, Leverkusen, Germany, Study-No.: 2012/01020e, Report date: 2012-07-24

3.3 Applicability domain (OECD principle 3)

a. Domains:

i. Molecular weight:

With a molecular weight of 706.15 g/mole bis(2-ethylhexyl) tetrabromophthalate is within the range of the training set (16 – 943 g/mole).

ii. **Structural fragment domain:**
Regarding the structure, the fragment descriptors used by the program for the estimation of the boiling point are complete and listed in Appendix F of the MPBPWIN help file.

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):

The structure of bis(2-ethylhexyl) tetrabromophthalate is not highly complex and the applied rules appear appropriate. An individual uncertainty for bis(2-ethylhexyl) tetrabromophthalate 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 vapour pressure yields a useful result for further evaluation.

4.4 Conclusion:

The result is considered as useful for regulatory purposes.

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