REACH

Propanamide, N-[2-(4-phenoxyphenoxy)ethyl]-

EC number: 600-606-0 | CAS number: 104825-66-3

Physical & Chemical properties

Boiling point

S-01 | Summary

Administrative data

Link to relevant study record(s)

Reference

Reference 1

Endpoint:	boiling point
Type of information:	(Q)SAR
Adequacy of study:	supporting study
Study period:	15-02-2018
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	results derived from a valid (Q)SAR model and falling into its applicability domain, with adequate and reliable documentation / justification
Remarks:	No QPRF is provided as model output
Justification for type of information:	1. SOFTWARE EPI Suite MPBPWIN v1.43 2. MODEL (incl. version number) MPBPWIN v1.43 3. SMILES OR OTHER IDENTIFIERS USED AS INPUT FOR THE MODEL c1(OCCNC(=O)CC)ccc(Oc2ccccc2)cc1 4. SCIENTIFIC VALIDITY OF THE (Q)SAR MODEL Please refer to the attached document taken directly from the help file of MPBPWIN v1.43 5. APPLICABILITY DOMAIN Please refer to the attached document taken directly from the help file of MPBPWIN v1.43 6. ADEQUACY OF THE RESULT No QPRF report was provided by the tool but the query substance falls within the applicability domain of the model.
Principles of method if other than guideline:	The normal boiling point is estimated in the MPBPWIN using an adaptation of the Stein and Brown (1994) method which is an extension and refinement of the Joback method (Joback, 1982; Reid et al, 1987).Please refer to the attached

	document for further information about the model methodology and validation.
GLP compliance:	no
Type of method:	other: QSAR model
Boiling pt.:	449.01 °C
Remarks on result:	other: QSAR result
The coefficient values for various contributing groups can be found in the attached prediction summary report.	
Executive summary:	The boiling point of propanamide, N-[2-(4-phenoxyphenoxy)ethyl]- was predicted as 449.01 °C using the EPI MPBPWIN v1.43. The substance was verified to fall within the applicability domain limits of the model.

Reference 2

Endpoint:	boiling point
Type of information:	(Q)SAR
Adequacy of study:	supporting study
Study period:	15-02-2018
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	results derived from a valid (Q)SAR model and falling into its applicability domain, with adequate and reliable documentation / justification
Remarks:	No QPRF was provided as model output. Only a prediction summary report was generated.
Justification for type of information:	1. SOFTWARE US EPA T.E.S.T (Toxicity Estimation Software Tool) v4.2.1 2. MODEL Normal Boiling Point model 3. SMILES OR OTHER IDENTIFIERS USED AS INPUT FOR THE MODEL c1(OCCNC(=O)CC)ccc(Oc2ccccc2)cc1 4. SCIENTIFIC VALIDITY OF THE (Q)SAR MODEL Please refer to the attached document: Page 35 of T.E.S.T User Guide 5. APPLICABILITY DOMAIN Please refer to the attached document: T.E.S.T User Guide 6. ADEQUACY OF THE RESULT No QPRF report was provided by the tool but the prediction was considered as reliable due to high structural similarity with the training set molecules.
Principles of method if other than guideline:	The boiling point prediction was derived as a consensus value from the following methods: a) Hierarchical clustering b) Group contribution c) Nearest Neighbor
GLP compliance:	no
Type of method:	other: QSAR result
Boiling pt.:	382.31 °C
Remarks on result:	other: QSAR result
The prediction was considered as reliable due to reasonable structural similarity with other training set substances. They are listed in a table provided in the prediction summary report. Moreover, the predictions with three different methodologies were comparable, therefore the consensus result was considered to be reliable.	
Executive summary:	The boiling point of propanamide, N-[2-(4-phenoxyphenoxy)ethyl]- was predicted as 382.31 °C using US EPA T.E.S.T v4.2.1. The prediction was considered as reliable due to high structural similarity with training set molecules. Moreover, the predictions with three different methodologies were comparable, therefore the consensus result was considered to be reliable.

Description of key information

The geometric mean of the boiling point predictions from two QSAR models was calculated.

Key value for chemical safety assessment

Boiling point at 101 325 Pa: 414.32 °C

Additional information

The geometric mean of the boiling point predictions from the following two QSAR models was considered:

a) EPISuite MPBPWIN v1.43 (Boiling Point predicted = 449.01°C)

b) US EPA T.E.S.T v4.2.1 (Boiling Point predicted = 382.31°C)