VEGA QSAR MODELS

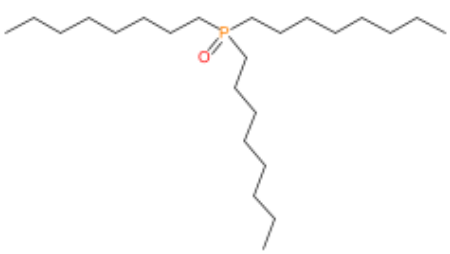
Report

Prediction and Applicability Domain analysis for models:

- Mutagenicity (Ames test) CONSENSUS model 1.0.4
- Mutagenicity (Ames test) model (CAESAR) 2.1.14
- Mutagenicity (Ames test) model (ISS) 1.0.3
- Mutagenicity (Ames test) model (SarPy-IRFMN) 1.0.8
- Mutagenicity (Ames test) model (KNN-Read-Across) 1.0.1
- Mutagenicity (Ames test) model for aromatic amines (CONCERT/IRFMN) 1.0.0
- Carcinogenicity model (CAESAR) 2.1.10
- Carcinogenicity model (ISS) 1.0.3
- Carcinogenicity model (IRFMN-ISSCAN-CGX) 1.0.2
- Carcinogenicity model (IRFMN-Antares) 1.0.2
- Carcinogenicity oral classification model (IRFMN) 1.0.1
- Carcinogenicity oral Slope Factor model (IRFMN) 1.0.1
- Carcinogenicity inhalation classification model (IRFMN) 1.0.1
- Carcinogenicity inhalation Slope Factor model (IRFMN) 1.0.1
- Carcinogenicity in male rat (CORAL) 1.0.0
- Carcinogenicity in female Rat (CORAL) 1.0.0
- Acute Toxicity (LD50) model (KNN) 1.0.0
- BCF model (CAESAR) 2.1.15
- BCF model (Meylan) 1.0.4
- BCF model (Arnot-Gobas) 1.0.1
- BCF model (KNN-Read-Across) 1.1.1

Core version: 1.3.18

Prediction for compound Molecule 0 -



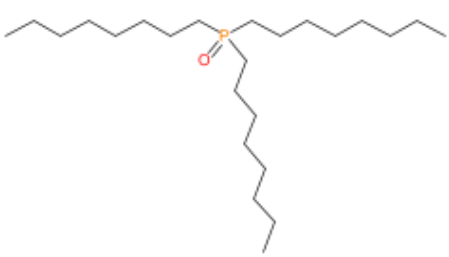
Prediction:

Prediction is NON-Mutagenic with a consensus score of 0.2, based on 4 models.

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Used models: 4
Predicted Consensus Mutagen activity: NON-Mutagenic
Mutagenic Score: 0
Non-Mutagenic Score: 0.2
Model Caesar assessment: NON-Mutagenic (LOW reliability)
Model ISS assessment: NON-Mutagenic (LOW reliability)
Model SarPy assessment: NON-Mutagenic (LOW reliability)
Model KNN assessment: NON-Mutagenic (LOW reliability)
Remarks:
none

1. Prediction Summary

Prediction for compound Molecule 0 -

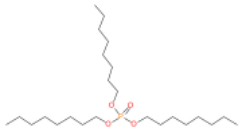


Prediction: Reliability:

Prediction is NON-Mutagenic, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Mutagen activity: NON-Mutagenic
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

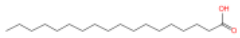


Compound #1

CAS: 1806-54-8
Dataset id:3666 (Training Set)
SMILES: O=P(OCCCCCCCCC)(OCCCCCCCCC)OCCCCCCCCC
Similarity: 0.752
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

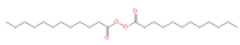
Compound #2

CAS: 112-92-5
Dataset id:596 (Training Set)
SMILES: OCCCCCCCCCCCCCCCCCC
Similarity: 0.75
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



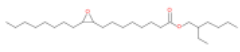
Compound #3

CAS: 57-11-4
Dataset id:3508 (Training Set)
SMILES: O=C(O)CCCCCCCCCCCCCCCCC
Similarity: 0.747
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #4

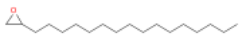
CAS: 105-74-8
Dataset id:1470 (Training Set)
SMILES: O=C(OOC(=O)CCCCCCCCCCC)CCCCCCCCCCC
Similarity: 0.738
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #5

CAS: 141-38-8
Dataset id:2569 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCCCCC1OC1(CCCCCCCC)
Similarity: 0.737
Experimental value : NON-Mutagenic
Predicted value : Suspect Mutagenic

Alerts (not found also in the target): SA7 Epoxides and aziridines



Compound #6

CAS: 7390-81-0
Dataset id:733 (Training Set)
SMILES: O1CC1CCCCCCCCCCCCCCC
Similarity: 0.732
Experimental value : NON-Mutagenic
Predicted value : Suspect Mutagenic

Alerts (not found also in the target): SA7 Epoxides and aziridines

3.2 Applicability Domain:
Measured Applicability Domain Scores

✗	Global AD Index AD index = 0.442 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.75 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✓	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✓	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✓	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✗	Atom Centered Fragments similarity check ACF index = 0.51 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)..

Symbols explanation:

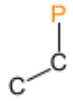
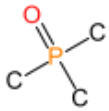
✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has less than 3 occurrences in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

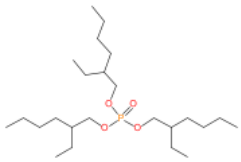
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is NON-Mutagenic, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

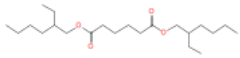
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Mutagen activity: NON-Mutagenic
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



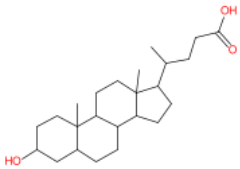
Compound #1

CAS: 78-42-2
Dataset id:69 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



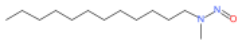
Compound #2

CAS: 103-23-1
Dataset id:52 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.697
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #3

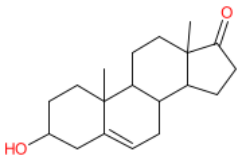
CAS: 434-13-9
Dataset id:117 (Training Set)
SMILES: O=C(O)CCC(C)C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.68
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #4

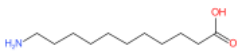
CAS: 55090-44-3
Dataset id:547 (Training Set)
SMILES: O=NN(C)CCCCCCCCCCCC
Similarity: 0.651
Experimental value : Mutagenic
Predicted value : Mutagenic

Alerts (not found also in the target): SA21 Alkyl and aryl N-nitroso groups



Compound #5

CAS: 53-43-0
Dataset id:836 (Training Set)
SMILES: O=C2CCC3C4CC=C1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.641
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #6

CAS: 2432-99-7
Dataset id:36 (Training Set)
SMILES: O=C(O)CCCCCCCCCCN
Similarity: 0.631
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

3.2 Applicability Domain:
Measured Applicability Domain Scores

✗	Global AD Index AD index = 0.336 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.705 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✓	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✓	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✗	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

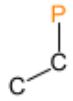
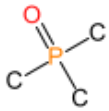
✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

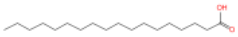
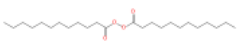
Prediction for compound Molecule 0 -

Prediction: Reliability:

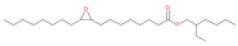
Prediction is NON-Mutagenic, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)
The following relevant fragments have been found: SM163; SM185

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Mutagen activity: NON-Mutagenic
No. alerts for mutagenicity: 0
No. alerts for non-mutagenicity: 2
Structural Alerts: SM163; SM185
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

	Compound #1 CAS: 1806-54-8 Dataset id:3666 (Training Set) SMILES: O=P(OCCCCCCCCC)(OCCCCCCCCC)OCCCCCCCCC Similarity: 0.752 Experimental value : NON-Mutagenic Predicted value : NON-Mutagenic Alerts (found also in the target): SM163 Alerts (not found also in the target): SM124
	Compound #2 CAS: 112-92-5 Dataset id:596 (Training Set) SMILES: OCCCCCCCCCCCCCCCCCC Similarity: 0.75 Experimental value : NON-Mutagenic Predicted value : NON-Mutagenic Alerts (found also in the target): SM163 Alerts (not found also in the target): SM157
	Compound #3 CAS: 57-11-4 Dataset id:3508 (Training Set) SMILES: O=C(O)CCCCCCCCCCCCCCCCC Similarity: 0.747 Experimental value : NON-Mutagenic Predicted value : NON-Mutagenic Alerts (found also in the target): SM163 Alerts (not found also in the target): SM143; SM157; SM177
	Compound #4 CAS: 105-74-8 Dataset id:1470 (Training Set) SMILES: O=C(OOC(=O)CCCCCCCCCCC)CCCCCCCCCCC Similarity: 0.738 Experimental value : NON-Mutagenic Predicted value : NON-Mutagenic Alerts (found also in the target): SM163 Alerts (not found also in the target): SM143; SM157; SM177

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

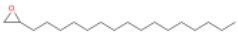


Compound #5

CAS: 141-38-8
Dataset id:2569 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCCCCC1OC1(CCCCCCCC)
Similarity: 0.737
Experimental value : NON-Mutagenic
Predicted value : Mutagenic

Alerts (found also in the target): SM163

Alerts (not found also in the target): SM97; SM123; SM143; SM157; SM169; SM177; SM178; SM182; SM188



Compound #6

CAS: 7390-81-0
Dataset id:733 (Training Set)
SMILES: O1CC1CCCCCCCCCCCCCCC
Similarity: 0.732
Experimental value : NON-Mutagenic
Predicted value : Mutagenic

Alerts (found also in the target): SM163

Alerts (not found also in the target): SM97; SM157

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.442 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.75 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✔	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✖	Atom Centered Fragments similarity check ACF index = 0.51 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)..

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.

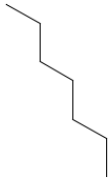
⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 1 of 2:.

Fragment found: SM163



Sarpy alert n. 163 for NON-Mutagenicity, defined by SMARTS: CCCCCCC

Following, the most similar compounds from the model's dataset having the same fragment.

CAS: 1806-54-8
Dataset id:3666 (Training Set)
SMILES: O=P(OCCCCCCCCC)(OCCCCCCCCC)OCCCCCCCCC
Similarity: 0.752

Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

Alerts (found also in the target): SM163

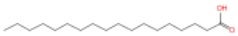
Alerts (not found also in the target): SM124

CAS: 112-92-5
Dataset id:596 (Training Set)
SMILES: OCCCCCCCCCCCCCCCCCC
Similarity: 0.75

Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

Alerts (found also in the target): SM163

Alerts (not found also in the target): SM157



CAS: 57-11-4
Dataset id:3508 (Training Set)
SMILES: O=C(O)CCCCCCCCCCCCCCCCCC
Similarity: 0.747

Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

Alerts (found also in the target): SM163

Alerts (not found also in the target): SM143; SM157; SM177

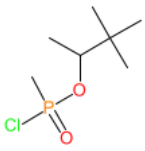
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 2 of 2:.

Fragment found: SM185

Sarpy alert n. 185 for NON-Mutagenicity, defined by SMARTS: PC

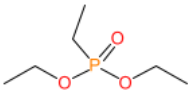
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 7040-57-5
Dataset id:3926 (Training Set)
SMILES: O=P(OC(C)C(C)(C)C)(C)Cl
Similarity: 0.557

Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

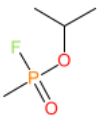
Alerts (found also in the target): SM185



CAS: 78-38-6
Dataset id:672 (Training Set)
SMILES: O=P(OCC)(OCC)CC
Similarity: 0.533

Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

Alerts (found also in the target): SM185



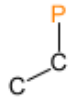
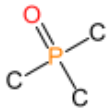
CAS: 107-44-8
Dataset id:2773 (Training Set)
SMILES: O=P(F)(OC(C)C)C
Similarity: 0.5

Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

Alerts (found also in the target): SM185

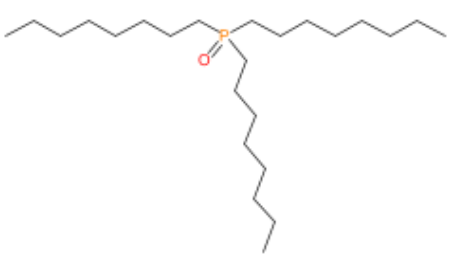
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has less than 3 occurrences in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

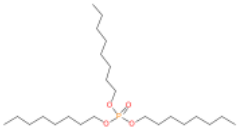
Prediction is NON-Mutagenic, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Mutagen activity: NON-Mutagenic
Molecules used for prediction: 4
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 557-61-9
Dataset id:3643 (Training Set)
SMILES: OCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Similarity: 0.762
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

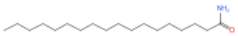


Compound #2

CAS: 1806-54-8
Dataset id:1965 (Training Set)
SMILES: O=P(OCCCCCCCC)(OCCCCCCCC)OCCCCCCCC
Similarity: 0.752
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

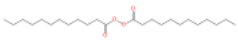
Compound #3

CAS: 112-92-5
Dataset id:620 (Training Set)
SMILES: OCCCCCCCCCCCCCCCCCC
Similarity: 0.75
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



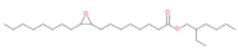
Compound #4

CAS: 124-26-5
Dataset id:962 (Training Set)
SMILES: O=C(N)CCCCCCCCCCCCCCCC
Similarity: 0.741
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #5

CAS: 105-74-8
Dataset id:238 (Training Set)
SMILES: O=C(OOC(=O)CCCCCCCCCCC)CCCCCCCCCCC
Similarity: 0.738
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #6

CAS: 141-38-8
Dataset id:1365 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCCCCC1OC1(CCCCCCCC)
Similarity: 0.737
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.442 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.751 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✔	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✖	Atom Centered Fragments similarity check ACF index = 0.51 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)..

Symbols explanation:

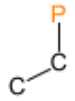
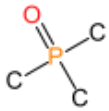
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

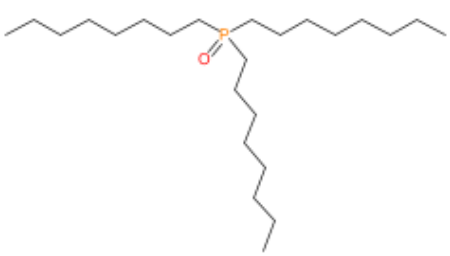
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has less than 3 occurrences in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0 -

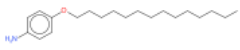


Prediction: Reliability:

Prediction is NA, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not adequate
- similar molecules found in the training set have experimental values that disagree with the predicted value
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

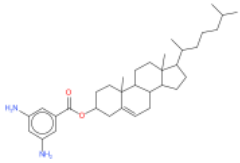
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Mutagen activity: NA
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



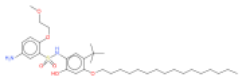
Compound #1

CAS: N.A.
Dataset id:6537 (Training Set)
SMILES: O(c1ccc(N)cc1)CCCCCCCCCCCCCC
Similarity: 0.676
Experimental value : NON-Mutagenic
Predicted value : Mutagenic



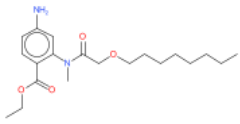
Compound #2

CAS: N.A.
Dataset id:7188 (Training Set)
SMILES:
O=C(OC4CC3=CCC1C(CCC2(C)(C(CCC12)C(C)CCCC(C)C))C3(C)CC4)c5cc(N)cc(N)c5
Similarity: 0.598
Experimental value : NON-Mutagenic
Predicted value : NA



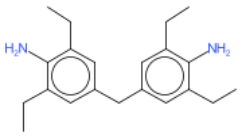
Compound #3

CAS: N.A.
Dataset id:4037 (Training Set)
SMILES:
O=S(=O)(Nc1cc(c(OCCCCCCCCCCCCCCCC)cc1(O))C(C)(C)C)c2cc(N)ccc2(OCCOC)
Similarity: 0.562
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



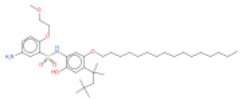
Compound #4

CAS: N.A.
Dataset id:7077 (Training Set)
SMILES: O=C(OCC)c1ccc(N)cc1N(C(=O)COCCCCCCCC)C
Similarity: 0.562
Experimental value : NON-Mutagenic
Predicted value : Mutagenic



Compound #5

CAS: N.A.
Dataset id:5101 (Training Set)
SMILES: Nc1c(cc(cc1CC)Cc2cc(c(N)c(c2)CC)CC)CC
Similarity: 0.559
Experimental value : NON-Mutagenic
Predicted value : Mutagenic



Compound #6

CAS: N.A.
Dataset id:6841 (Training Set)
SMILES:
O=S(=O)(Nc1cc(OCCCCCCCCCCCCCCCCC)c(cc1(O))C(C)(C)CC(C)(C)C)c2cc(N)ccc2(OCCOC)
Similarity: 0.555
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.633 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✖	Accuracy of prediction for similar molecules Accuracy index = 0 Explanation: Accuracy of prediction for similar molecules found in the training set is not adequate..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✖	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

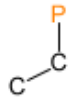
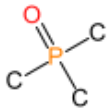
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

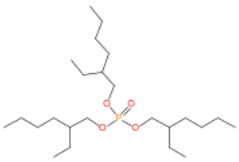
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is NON-Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

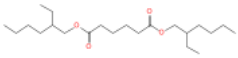
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Carcinogen activity: NON-Carcinogen
P(Carcinogen): 0.13
P(NON-Carcinogen): 0.87
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 78-42-2
Dataset id:784 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

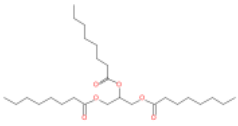


Compound #2

CAS: 103-23-1
Dataset id:315 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.697
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

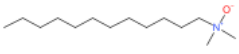
Compound #3

CAS: 112-63-0
Dataset id:451 (Test Set)
SMILES: O=C(OC)CCCCCCCC=CCC=CCCCCC
Similarity: 0.695
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



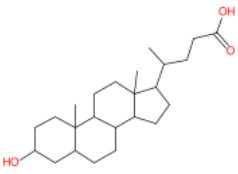
Compound #4

CAS: 538-23-8
Dataset id:759 (Test Set)
SMILES: O=C(OCC(OC(=O)CCCCCCC)COC(=O)CCCCCCC)CCCCCCC
Similarity: 0.683
Experimental value : Carcinogen
Predicted value : NON-Carcinogen



Compound #5

CAS: 1643-20-5
Dataset id:273 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.681
Experimental value : NON-Carcinogen
Predicted value : Carcinogen



Compound #6

CAS: 434-13-9
Dataset id:413 (Training Set)
SMILES: O=C(O)CCC(C)C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.68
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✗	Global AD Index AD index = 0.336 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.705 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✓	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✓	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✓	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✗	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..
✓	Model class assignment reliability Pos/Non-Pos difference = 0.739 Explanation: model class assignment is well defined..
✓	Neural map neurons concordance Neurons concordance = 1 Explanation: predicted value agrees with experimental values of training set compounds laying in the same neuron..

Symbols explanation:

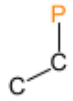
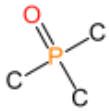
✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

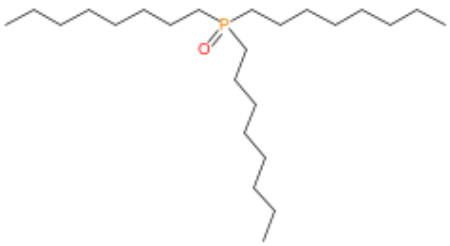
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0 -

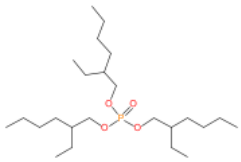


Prediction: Reliability:

Prediction is NON-Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Carcinogen activity: NON-Carcinogen
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

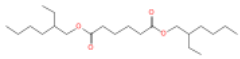
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 78-42-2
Dataset id:69 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : Carcinogen
Predicted value : Carcinogen

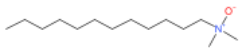
Alerts (not found also in the target): SA41 Substituted n-alkylcarboxylic acids



Compound #2

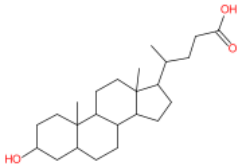
CAS: 103-23-1
Dataset id:52 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.697
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): SA41 Substituted n-alkylcarboxylic acids; SA42 Phthalate diesters and monoesters



Compound #3

CAS: 1643-20-5
Dataset id:879 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.681
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #4

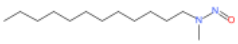
CAS: 434-13-9
Dataset id:117 (Training Set)
SMILES: O=C(O)CCC(C)C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.68
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #5

CAS: 75881-20-8
Dataset id:579 (Training Set)
SMILES: O=NN(C)CCCCCCCCCCCCCC
Similarity: 0.675
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): SA21 Alkyl and aryl N-nitroso groups

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 55090-44-3
Dataset id:547 (Training Set)
SMILES: O=NN(C)CCCCCCCCCCCC
Similarity: 0.651
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): SA21 Alkyl and aryl N-nitroso groups

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.705 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✖	Atom Centered Fragments similarity check ACF index = 0.51 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)..

Symbols explanation:

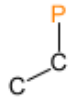
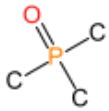
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has less than 3 occurrences in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

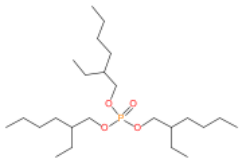
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is Possible NON-Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Carcinogenic activity: Possible NON-Carcinogen
No. alerts for carcinogenicity: 0
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

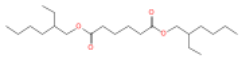
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 78-42-2
Dataset id:59 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : Carcinogen
Predicted value : Carcinogen

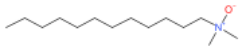
Alerts (not found also in the target): Carcinogenity alert no. 15



Compound #2

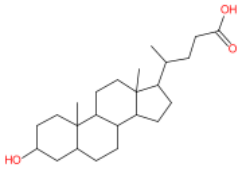
CAS: 103-23-1
Dataset id:43 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.697
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 29



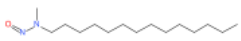
Compound #3

CAS: 1643-20-5
Dataset id:777 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.681
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen



Compound #4

CAS: 434-13-9
Dataset id:93 (Training Set)
SMILES: O=C(O)CCC(C)C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.68
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

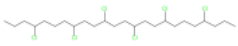


Compound #5

CAS: 75881-20-8
Dataset id:489 (Training Set)
SMILES: O=NN(C)CCCCCCCCCCCCCC
Similarity: 0.675
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 1; Carcinogenity alert no. 14; Carcinogenity alert no. 27

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 63449-39-8
Dataset id:810 (Training Set)
SMILES: CCCC(CCCC(CCC(CCC(CCC(CCCC(CCC)Cl)Cl)Cl)Cl)Cl)Cl
Similarity: 0.654
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 18

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.32 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.697 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✖	Concordance for similar molecules Concordance index = 0.321 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✖	Atom Centered Fragments similarity check ACF index = 0.51 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent_fragments found)..

Symbols explanation:

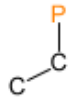
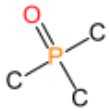
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has less than 3 occurrences in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

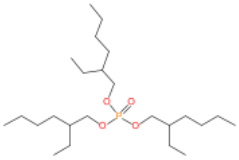
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is Possible NON-Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not optimal
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Carcinogenic activity: Possible NON-Carcinogen
No. alerts for carcinogenicity: 0
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

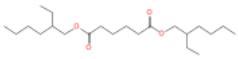
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 78-42-2
Dataset id:784 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : NON-Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 98

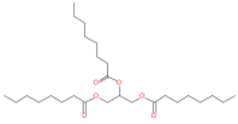


Compound #2

CAS: 103-23-1
Dataset id:315 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.697
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

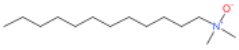
Compound #3

CAS: 112-63-0
Dataset id:451 (Test Set)
SMILES: O=C(OC)CCCCCCCC=CCC=CCCCCC
Similarity: 0.695
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen



Compound #4

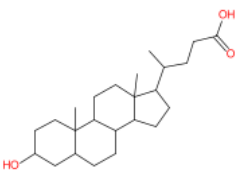
CAS: 538-23-8
Dataset id:759 (Test Set)
SMILES: O=C(OCC(OC(=O)CCCCCCC)COC(=O)CCCCCCC)CCCCCCC
Similarity: 0.683
Experimental value : Carcinogen
Predicted value : Possible NON-Carcinogen



Compound #5

CAS: 1643-20-5
Dataset id:273 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.681
Experimental value : NON-Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 64



Compound #6

CAS: 434-13-9
Dataset id:413 (Training Set)
SMILES: O=C(O)CCC(C)C2CCC3C4CCC1CC(O)CCC1(C)C4(CCC23(C))
Similarity: 0.68
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.302 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.702 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
⚠	Accuracy of prediction for similar molecules Accuracy index = 0.658 Explanation: Accuracy of prediction for similar molecules found in the training set is not optimal..
✔	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✖	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

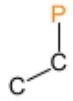
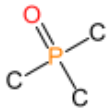
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

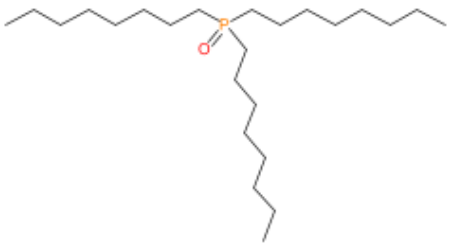
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0 -

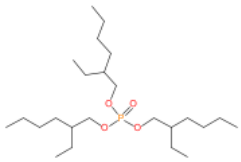


Prediction: Reliability:

Prediction is Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not adequate
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found)

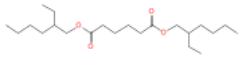
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Oral Carcinogenic class: Carcinogen
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



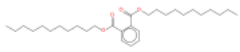
Compound #1

CAS: 78-42-2
Dataset id:313 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : Carcinogen
Predicted value : Carcinogen



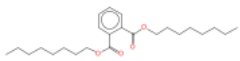
Compound #2

CAS: 103-23-1
Dataset id:94 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.697
Experimental value : Carcinogen
Predicted value : NON-Carcinogen



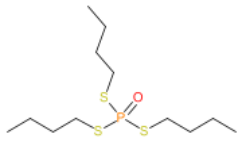
Compound #3

CAS: 3648-20-2
Dataset id:488 (Training Set)
SMILES: O=C(OCCCCCCCCCCC)c1ccccc1(C(=O)OCCCCCCCCCCC)
Similarity: 0.673
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



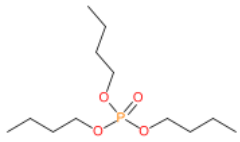
Compound #4

CAS: 117-84-0
Dataset id:614 (Training Set)
SMILES: O=C(OCCCCCCCC)c1ccccc1(C(=O)OCCCCCCCC)
Similarity: 0.65
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #5

CAS: 78-48-8
Dataset id:568 (Training Set)
SMILES: O=P(SCCCC)(SCCCC)SCCCC
Similarity: 0.639
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #6

CAS: 126-73-8
Dataset id:299 (Training Set)
SMILES: O=P(OCCCC)(OCCCC)OCCCC
Similarity: 0.627
Experimental value : Carcinogen
Predicted value : Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.426 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.705 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✖	Accuracy of prediction for similar molecules Accuracy index = 0.509 Explanation: Accuracy of prediction for similar molecules found in the training set is not adequate..
✔	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✖	Atom Centered Fragments similarity check ACF index = 0.6 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found)..

Symbols explanation:

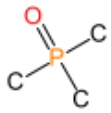
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

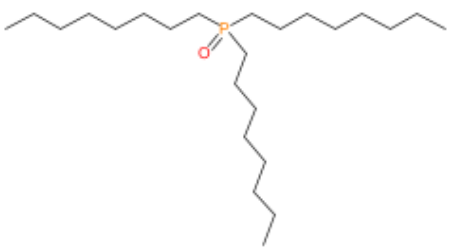
(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:



Fragment defined by the SMILES: CP(C)(C)=O
The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0 -

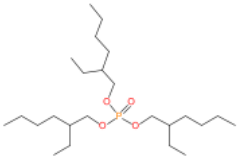


Prediction: Reliability:

Prediction is -1.79, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- some similar molecules found in the training set have experimental values that disagree with the predicted value
- the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

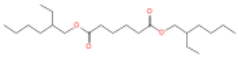
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Oral Carcinogenicity SF (log form) [log(1/(mg/kg-day))]: -1.79
Predicted Oral Carcinogenicity SF [1/(mg/kg-day)]: 0.0161
Experimental value [1/(mg/kg-day)]: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



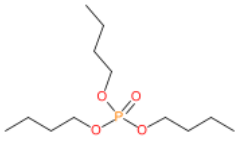
Compound #1

CAS: 78-42-2
Dataset id:313 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : -2.49
Predicted value : -2.174



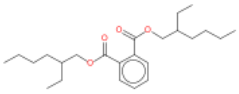
Compound #2

CAS: 103-23-1
Dataset id:94 (Test Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.697
Experimental value : -2.92
Predicted value : -1.999



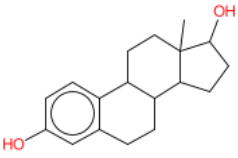
Compound #3

CAS: 126-73-8
Dataset id:299 (Training Set)
SMILES: O=P(OCCCC)(OCCCC)OCCCC
Similarity: 0.627
Experimental value : -2.05
Predicted value : -2.145



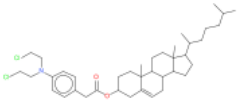
Compound #4

CAS: 117-81-7
Dataset id:44 (Test Set)
SMILES: O=C(OCC(CC)CCCC)c1ccccc1(C(=O)OCC(CC)CCCC)
Similarity: 0.626
Experimental value : -1.85
Predicted value : -2.919



Compound #5

CAS: 50-28-2
Dataset id:141 (Training Set)
SMILES: Oc1ccc2c(c1)CCC3C2CCC4(C)(C(O)CCC34)
Similarity: 0.586
Experimental value : 1.59
Predicted value : 0.663



Compound #6

CAS: 3546-10-9
Dataset id:256 (Training Set)
SMILES:
O=C(OC4CC3=CCC1C(CCC2(C)(C(CCC12)C(C)CCCC(C)C))C3(C)CC4)Cc5ccc(cc5)N(CCCl)CCCl
Similarity: 0.572
Experimental value : 2.18
Predicted value : 0.78

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.282 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.705 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 0.618 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
⚠	Concordance for similar molecules Concordance index = 0.911 Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value..
⚠	Maximum error of prediction among similar molecules Max error index = 0.921 Explanation: the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✖	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

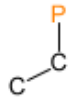
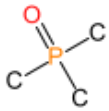
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

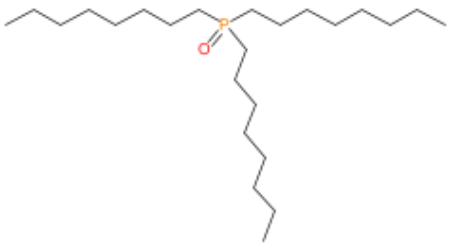
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0 -

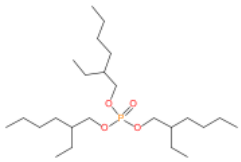


Prediction: Reliability:

Prediction is Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found)

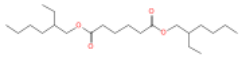
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Inhalation Carcinogenic class: Carcinogen
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



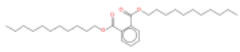
Compound #1

CAS: 78-42-2
Dataset id:741 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



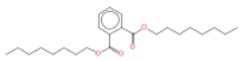
Compound #2

CAS: 103-23-1
Dataset id:391 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.697
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



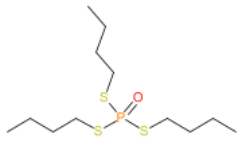
Compound #3

CAS: 3648-20-2
Dataset id:460 (Test Set)
SMILES: O=C(OCCCCCCCCCCC)c1ccccc1(C(=O)OCCCCCCCCCCC)
Similarity: 0.673
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



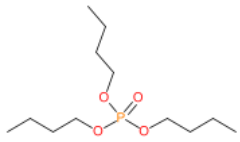
Compound #4

CAS: 117-84-0
Dataset id:597 (Training Set)
SMILES: O=C(OCCCCCCCC)c1ccccc1(C(=O)OCCCCCCCC)
Similarity: 0.65
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #5

CAS: 78-48-8
Dataset id:547 (Training Set)
SMILES: O=P(SCCCC)(SCCCC)SCCCC
Similarity: 0.639
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #6

CAS: 126-73-8
Dataset id:708 (Training Set)
SMILES: O=P(OCCCC)(OCCCC)OCCCC
Similarity: 0.627
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.705 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✖	Atom Centered Fragments similarity check ACF index = 0.6 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found)..

Symbols explanation:

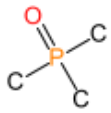
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:



Fragment defined by the SMILES: CP(C)(C)=O
The fragment has never been found in the model's training set

1. Prediction Summary

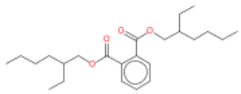
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is 0.14, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- No similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not optimal
- similar molecules found in the training set have experimental values that disagree with the predicted value
- the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

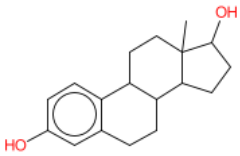
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted Inhalation Carcinogenicity SF (log form) [log(1/(mg/kg-day))]: 0.14
Predicted Inhalation Carcinogenicity SF [1/(mg/kg-day)]: 1.37
Experimental value [1/(mg/kg-day)]: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



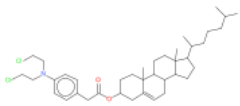
Compound #1

CAS: 117-81-7
Dataset id:38 (Training Set)
SMILES: O=C(OCC(CC)CCCC)c1ccccc1(C(=O)OCC(CC)CCCC)
Similarity: 0.626
Experimental value : -2.08
Predicted value : 0.163



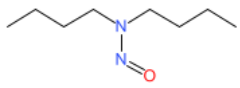
Compound #2

CAS: 50-28-2
Dataset id:116 (Training Set)
SMILES: Oc1ccc2c(c1)CCC3C2CCC4(C)(C(O)CCC34)
Similarity: 0.586
Experimental value : 1.59
Predicted value : 2.033



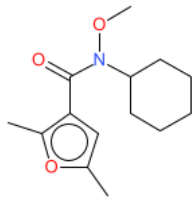
Compound #3

CAS: 3546-10-9
Dataset id:219 (Test Set)
SMILES:
O=C(OC4CC3=CCC1C(CCC2(C)(C(CCC12)C(C)CCCC(C)C))C3(C)CC4)Cc5ccc(cc5)N(CCCl)CCCl
Similarity: 0.572
Experimental value : 2.18
Predicted value : 1.825



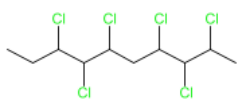
Compound #4

CAS: 924-16-3
Dataset id:192 (Training Set)
SMILES: O=NN(CCCC)CCCC
Similarity: 0.557
Experimental value : 0.75
Predicted value : -0.335



Compound #5

CAS: 60568-05-0
Dataset id:123 (Training Set)
SMILES: O=C(c1cc(oc1C)C)N(OC)C2CCCCC2
Similarity: 0.556
Experimental value : -1.52
Predicted value : 0.268



Compound #6

CAS: 108171-26-2
Dataset id:54 (Training Set)
SMILES: CCC(C(C(CC(C(C(C)Cl)Cl)Cl)Cl)Cl)Cl
Similarity: 0.547
Experimental value : -1.06
Predicted value : 0.58

3.2 Applicability Domain:
Measured Applicability Domain Scores

✗	Global AD Index AD index = 0.242 Explanation: The predicted compound is outside the Applicability Domain of the model.
✗	Similar molecules with known experimental value Similarity index = 0.605 Explanation: No similar compounds with known experimental value in the training set have been found..
⚠	Accuracy of prediction for similar molecules Accuracy index = 1.343 Explanation: Accuracy of prediction for similar molecules found in the training set is not optimal..
✗	Concordance for similar molecules Concordance index = 1.835 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✗	Maximum error of prediction among similar molecules Max error index = 2.243 Explanation: the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability..
✓	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✗	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

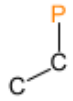
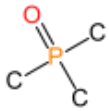
✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

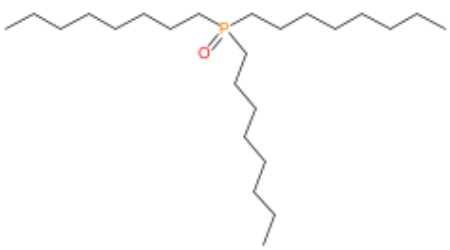
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0 -

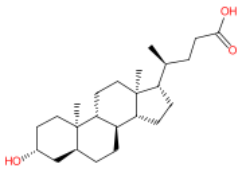


Prediction: Reliability:

Prediction is -2.0945, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- No similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not adequate
- the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

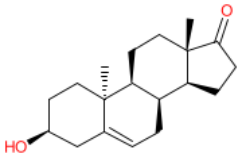
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted TD50 [-log(mg/kg bw/day)]: -2.0945
Predicted TD50 [mg/kg bw/day]: 124.3
Experimental TD50 [mg/kg bw/day]: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



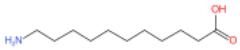
Compound #1

CAS: N.A.
Dataset id:129 (Training Set)
SMILES:
[C@@H]1(C[C@H]2[C@@](CC1)([C@H]1[C@H](CC2)[C@@H]2[C@@](CC1)([C@@H](CC2)[C@@H](C)CCC(=O)O)C)C)O
Similarity: 0.68
Experimental value : -3.352
Predicted value : -0.763



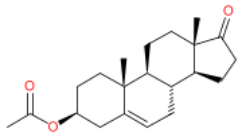
Compound #2

CAS: N.A.
Dataset id:164 (Test Set)
SMILES:
C12=CC[C@H]3[C@@H]([C@@]2(CC[C@@H](C1)O)C)CC[C@]1([C@H]3CCC1=O)C
Similarity: 0.641
Experimental value : -1.833
Predicted value : -0.788



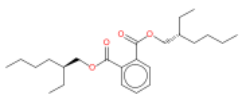
Compound #3

CAS: N.A.
Dataset id:34 (Training Set)
SMILES: C(CCCCCCCCCC(=O)O)N
Similarity: 0.631
Experimental value : -3.041
Predicted value : -2.357



Compound #4

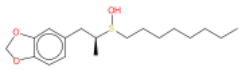
CAS: N.A.
Dataset id:81 (Training Set)
SMILES:
[C@H]1(CC2=CC[C@@H]3[C@@H]([C@]2(CC1)C)CC[C@]1([C@H]3CCC1=O)C)OC(=O)C
Similarity: 0.631
Experimental value : -1.559
Predicted value : -1.497



Compound #5

CAS: N.A.
Dataset id:122 (Training Set)
SMILES: c1ccc(c(c1)C(=O)OC[C@H](CCCC)CC)C(=O)OC[C@@H](CCCC)CC
Similarity: 0.626
Experimental value : -3.068
Predicted value : -2.992

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: N.A.
Dataset id:132 (Training Set)
SMILES: c12c(cc(cc1)C[C@H](C)[S@@](CCCCCCCC)O)OCO2
Similarity: 0.609
Experimental value : -3.423
Predicted value : -1.206

3.2 Applicability Domain:
Measured Applicability Domain Scores

✗	Global AD Index AD index = 0.264 Explanation: The predicted compound is outside the Applicability Domain of the model.
✗	Similar molecules with known experimental value Similarity index = 0.659 Explanation: No similar compounds with known experimental value in the training set have been found..
✗	Accuracy of prediction for similar molecules Accuracy index = 1.817 Explanation: Accuracy of prediction for similar molecules found in the training set is not adequate..
✓	Concordance for similar molecules Concordance index = 0.76 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✗	Maximum error of prediction among similar molecules Max error index = 2.589 Explanation: the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability..
✓	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✗	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

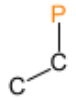
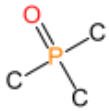
✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

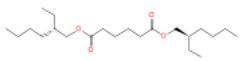
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is -1.5974, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- No similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not optimal
- similar molecules found in the training set have experimental values that disagree with the predicted value
- the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

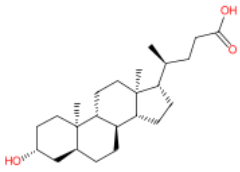
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted TD50 [-log(mg/kg bw/day)]: -1.5974
Predicted TD50 [mg/kg bw/day]: 39.57
Experimental TD50 [mg/kg bw/day]: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



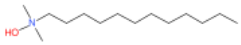
Compound #1

CAS: N.A.
Dataset id:113 (Training Set)
SMILES: CCCC[C@H](CC)COC(=O)CCCCC(=O)OC[C@H](CC)CCCC
Similarity: 0.697
Experimental value : -4.161
Predicted value : -2.71



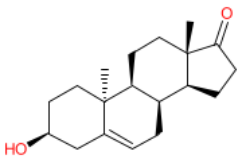
Compound #2

CAS: N.A.
Dataset id:47 (Training Set)
SMILES:
[C@@H]1(C[C@H]2[C@@](CC1)([C@H]1[C@H](CC2)[C@@H]2[C@@](CC1)([C@@H](CC2)[C@@H](C)CCC(=O)O)C)C)O
Similarity: 0.68
Experimental value : -3.276
Predicted value : -4.644



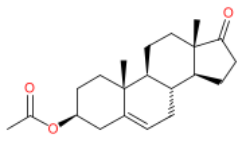
Compound #3

CAS: N.A.
Dataset id:93 (Training Set)
SMILES: CCCCCCCCCCCC[N](O)(C)C
Similarity: 0.68
Experimental value : -2.364
Predicted value : -0.843



Compound #4

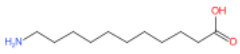
CAS: N.A.
Dataset id:25 (Training Set)
SMILES:
C12=CC[C@H]3[C@@H]([C@@]2(CC[C@@H](C1)O)C)CC[C@]1([C@H]3CCC1=O)C
Similarity: 0.641
Experimental value : -1.921
Predicted value : -4.971



Compound #5

CAS: N.A.
Dataset id:33 (Training Set)
SMILES:
[C@H]1(CC2=CC[C@@H]3[C@@H]([C@]2(CC1)C)CC[C@]1([C@H]3CCC1=O)C)OC(=O)C
Similarity: 0.631
Experimental value : -2.362
Predicted value : -1.307

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: N.A.
Dataset id:117 (Training Set)
SMILES: C(CCCCCCCCCC(=O)O)N
Similarity: 0.631
Experimental value : -4.649
Predicted value : -4.782

3.2 Applicability Domain:
Measured Applicability Domain Scores

✗	Global AD Index AD index = 0.275 Explanation: The predicted compound is outside the Applicability Domain of the model.
✗	Similar molecules with known experimental value Similarity index = 0.688 Explanation: No similar compounds with known experimental value in the training set have been found..
⚠	Accuracy of prediction for similar molecules Accuracy index = 1.41 Explanation: Accuracy of prediction for similar molecules found in the training set is not optimal..
✗	Concordance for similar molecules Concordance index = 2.121 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
⚠	Maximum error of prediction among similar molecules Max error index = 1.451 Explanation: the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability..
✓	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✗	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

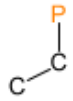
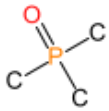
✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

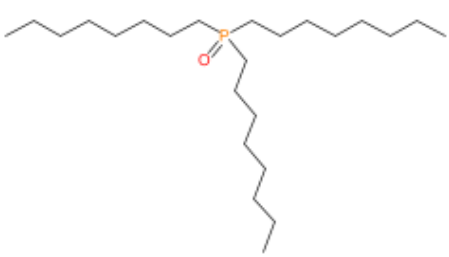
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0 -

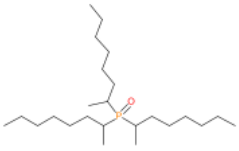


Prediction: Reliability:

Prediction is 9641.98 mg/kg, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.

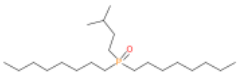
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted log LD50 [log(mmol/Kg)]: 1.397
Predicted log LD50 [mg/Kg]: 9641.98
Molecules used for prediction: 3
Experimental value [mg/Kg]: -
Reliability: The predicted compound is into the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: N.A.
Dataset id:2782 (Training Set)
SMILES: O=P(C(C)CCCCCC)(C(C)CCCCCC)C(C)CCCCCC
Similarity: 0.988
Experimental value : 1.27
Predicted value : 1.324

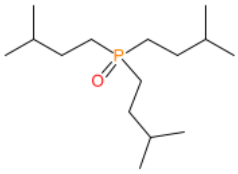


Compound #2

CAS: N.A.
Dataset id:2575 (Training Set)
SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCC(C)C
Similarity: 0.958
Experimental value : 1.39
Predicted value : 1.266

Compound #3

CAS: N.A.
Dataset id:2480 (Training Set)
SMILES: O=P(OC)(OC)CCCCCCCCCCCCCCCCCC
Similarity: 0.819
Experimental value : 1.63
Predicted value : 1.2



Compound #4

CAS: N.A.
Dataset id:1696 (Training Set)
SMILES: O=P(CCC(C)C)(CCC(C)C)CCC(C)C
Similarity: 0.795
Experimental value : 0.93
Predicted value : 0.807

Compound #5

CAS: N.A.
Dataset id:2664 (Training Set)
SMILES: OCCCCCCCCCCCCCCCCCCCCC
Similarity: 0.774
Experimental value : 1.49
Predicted value : 1.6

Compound #6

CAS: N.A.
Dataset id:5641 (Training Set)
SMILES: OCCCCCCCCCCCCCCCCCCCC
Similarity: 0.768
Experimental value : 1.53
Predicted value : 1.587

3.2 Applicability Domain:
Measured Applicability Domain Scores

✓	Global AD Index AD index = 1 Explanation: The predicted compound is into the Applicability Domain of the model.
✓	Similar molecules with known experimental value Similarity index = 0.895 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
✓	Accuracy of prediction for similar molecules Accuracy index = 0.203 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✓	Concordance for similar molecules Concordance index = 0.122 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✓	Maximum error of prediction among similar molecules Max error index = 0.43 Explanation: the maximum error in prediction of similar molecules found in the training set has a low value, considering the experimental variability..
✓	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

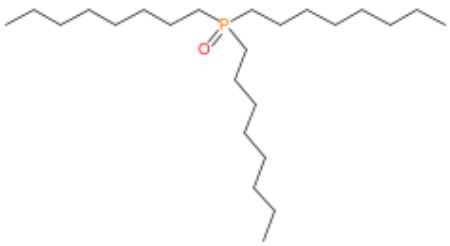
✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

Prediction is 1.07 log(L/kg), but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- No similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted BCF [log(L/kg)]: 1.07
Predicted BCF [L/kg]: 12
Predicted BCF from sub-model 1 (HM) [log(L/kg)]: 1.29
Predicted BCF from sub-model 2 (GA) [log(L/kg)]: 1.27
Predicted LogP (MLogP): 7.08
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

2. Possible Use and Uncertainty

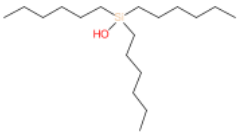
Threshold 3.3 (bioaccumulative)

Following, a chart showing the predicted value together with its conservative confidence interval for safe classification.
For the threshold logBCF = 3.3, the current compound can not be associated (due to its Applicability Domain index value) to any conservative interval.
No safe classification can be done.

Threshold 3.7 (very bioaccumulative)

Following, a chart showing the predicted value together with its conservative confidence interval for safe classification.
For the threshold logBCF = 3.7, the current compound can not be associated (due to its Applicability Domain index value) to any conservative interval.
No safe classification can be done.

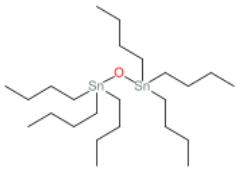
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 60782-58-3
Dataset id:465 (Training Set)
SMILES: O[Si](CCCCCC)(CCCCCC)CCCCCC
Similarity: 0.726
Experimental value : 1.48
Predicted value : 1.927

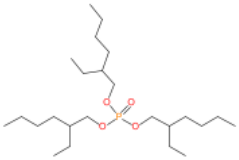
Alerts (not found also in the target): Si atom in the molecule (SO 03); OH group (PG 06)



Compound #2

CAS: 56-35-9
Dataset id:466 (Training Set)
SMILES: O([Sn](CCCC)(CCCC)CCCC)[Sn](CCCC)(CCCC)CCCC
Similarity: 0.715
Experimental value : 3.85
Predicted value : 3.686

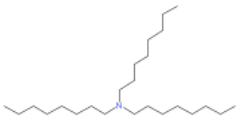
Alerts (not found also in the target): Sn atom in the molecule (SO 04)



Compound #3

CAS: 78-42-2
Dataset id:405 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : 1.19
Predicted value : 1.31

Alerts (not found also in the target): PO2 residue (SR 03)



Compound #4

CAS: 1116-76-3
Dataset id:306 (Training Set)
SMILES: N(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Similarity: 0.712
Experimental value : 1.92
Predicted value : 1.35

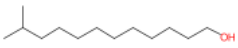
Alerts (not found also in the target): Tertiary amine (SR 05)

Compound #5

CAS: 28299-29-8
Dataset id:290 (Training Set)
SMILES: O=C(O)CC(C(=O)O)CCCCCCCCC=CCCCCCCCC
Similarity: 0.702
Experimental value : 0.22
Predicted value : 0.993

Alerts (not found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 27458-92-0
Dataset id:11 (Training Set)
SMILES: OCCCCCCCCCCC(C)C
Similarity: 0.686
Experimental value : 2.73
Predicted value : 2.259

Alerts (not found also in the target): OH group (PG 06)

3.2 Applicability Domain:
Measured Applicability Domain Scores

✗	Global AD Index AD index = 0.288 Explanation: The predicted compound is outside the Applicability Domain of the model.
✗	Similar molecules with known experimental value Similarity index = 0.72 Explanation: No similar compounds with known experimental value in the training set have been found..
✓	Accuracy of prediction for similar molecules Accuracy index = 0.306 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✗	Concordance for similar molecules Concordance index = 1.59 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✓	Maximum error of prediction among similar molecules Max error index = 0.447 Explanation: the maximum error in prediction of similar molecules found in the training set has a low value, considering the experimental variability..
✓	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✗	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

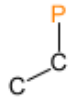
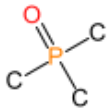
✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

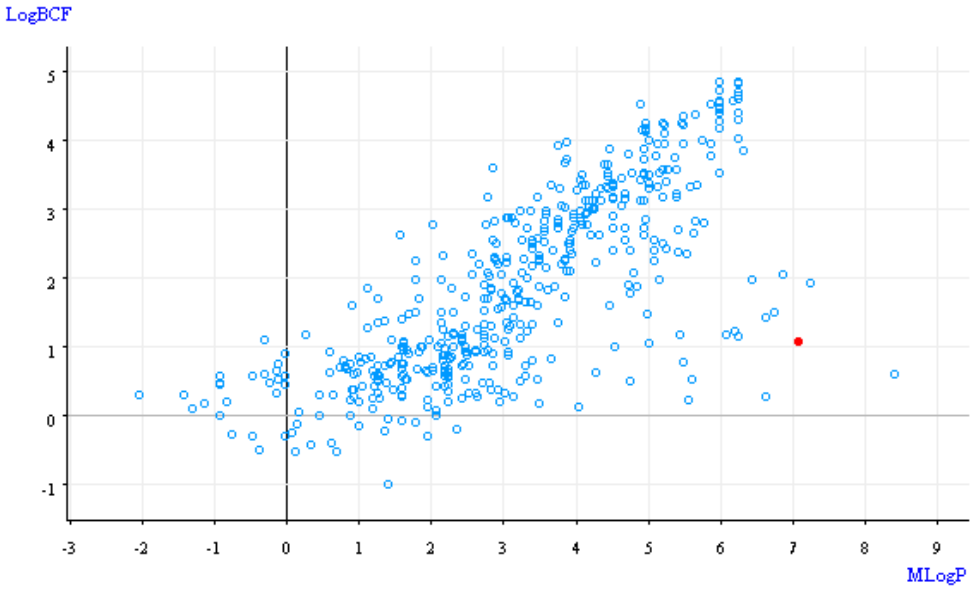
(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

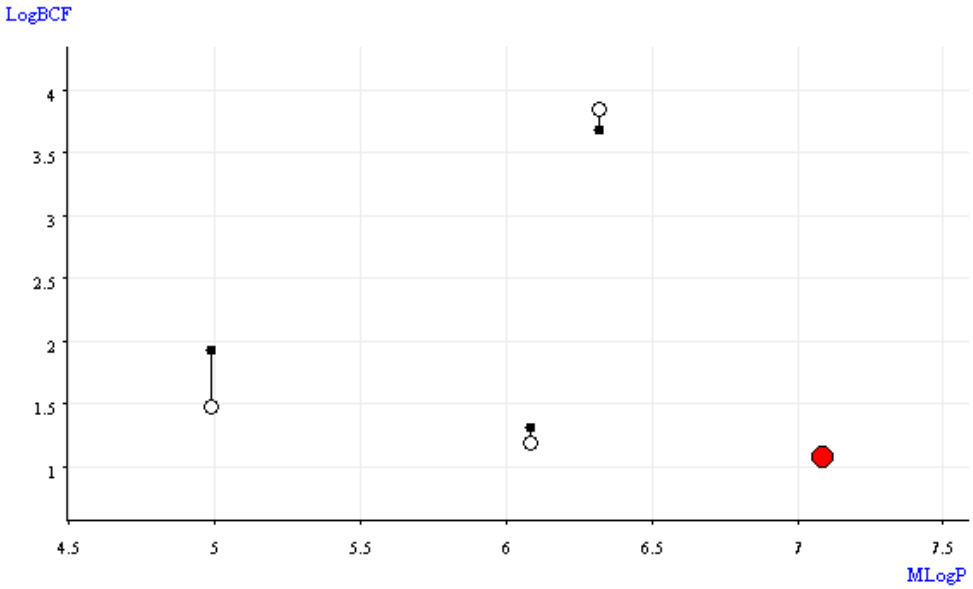
4.2 Reasoning:
Analysis of Molecular Descriptors

Descriptor name: MLogP
Descriptor name: LogP is directly correlated to the logBCF value.

Following, a scatterplot of MLogP against response values; experimental values are reported for the training set, predicted value for the studied compound. Light blue dots represent values of compounds from training set, red dot is the value of the studied compound.



Following, a scatterplot of MLogP against response values only for 3 most similar compounds in the training set. Red dot is the value of the studied compound, black outlined circles represents experimental values of compounds from training set, black dots represents predicted value of the same compound; the size of the circle is proportional to the similarity to the studied compound.



1. Prediction Summary

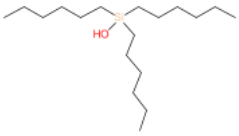
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is 2.18 log(L/kg), but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- No similar compounds with known experimental value in the training set have been found
- the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability
- reliability of logP value used by the model is not optimal
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

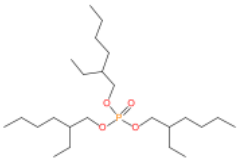
Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted BCF [log(L/kg)]: 2.18
Predicted BCF [L/kg]: 150
Predicted LogP (Meylan/Kowwin): 9.76
Predicted LogP reliability: Moderate
MW: 384.23
Ionic compound: no
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



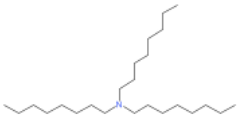
Compound #1

CAS: 60782-58-3
Dataset id:518 (Training Set)
SMILES: O[Si](CCCCCC)(CCCCCC)CCCCCC
Similarity: 0.726
Experimental value : 2.7
Predicted value : 2.098



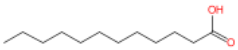
Compound #2

CAS: 78-42-2
Dataset id:522 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : 1.7
Predicted value : 1.482



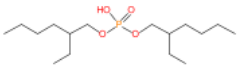
Compound #3

CAS: 1116-76-3
Dataset id:647 (Test Set)
SMILES: N(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Similarity: 0.712
Experimental value : 1.93
Predicted value : 2.482



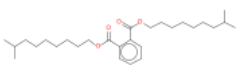
Compound #4

CAS: 629-25-4
Dataset id:30 (Training Set)
SMILES: O=C(O)CCCCCCCCCCC
Similarity: 0.675
Experimental value : 2.4
Predicted value : 0.5



Compound #5

CAS: 298-07-7
Dataset id:633 (Test Set)
SMILES: O=P(O)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.667
Experimental value : 0.64
Predicted value : 1.473



Compound #6

CAS: 26761-40-0
Dataset id:525 (Training Set)
SMILES: O=C(OCCCCCCCCC(C)C)c1ccccc1(C(=O)OCCCCCCCCC(C)C)
Similarity: 0.654
Experimental value : 1.16
Predicted value : 2.479

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.288 Explanation: The predicted compound is outside the Applicability Domain of the model.
✖	Similar molecules with known experimental value Similarity index = 0.72 Explanation: No similar compounds with known experimental value in the training set have been found..
✔	Accuracy of prediction for similar molecules Accuracy index = 0.41 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✔	Concordance for similar molecules Concordance index = 0.5 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
⚠	Maximum error of prediction among similar molecules Max error index = 0.602 Explanation: the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability..
⚠	Reliability of logP prediction LogP reliability = 0.7 Explanation: reliability of logP value used by the model is not optimal..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the defined range..
✖	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

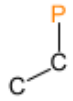
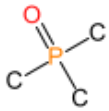
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

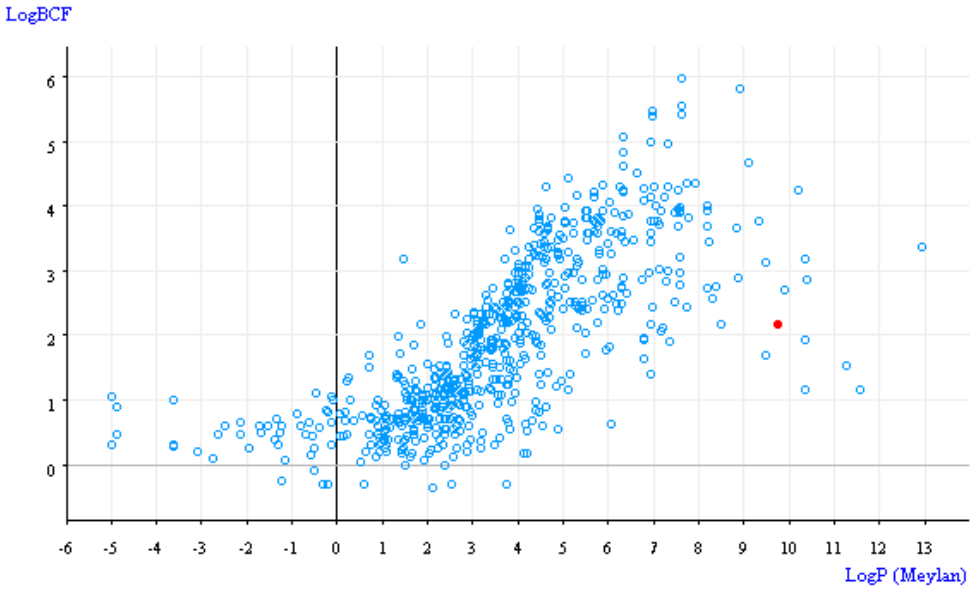
(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

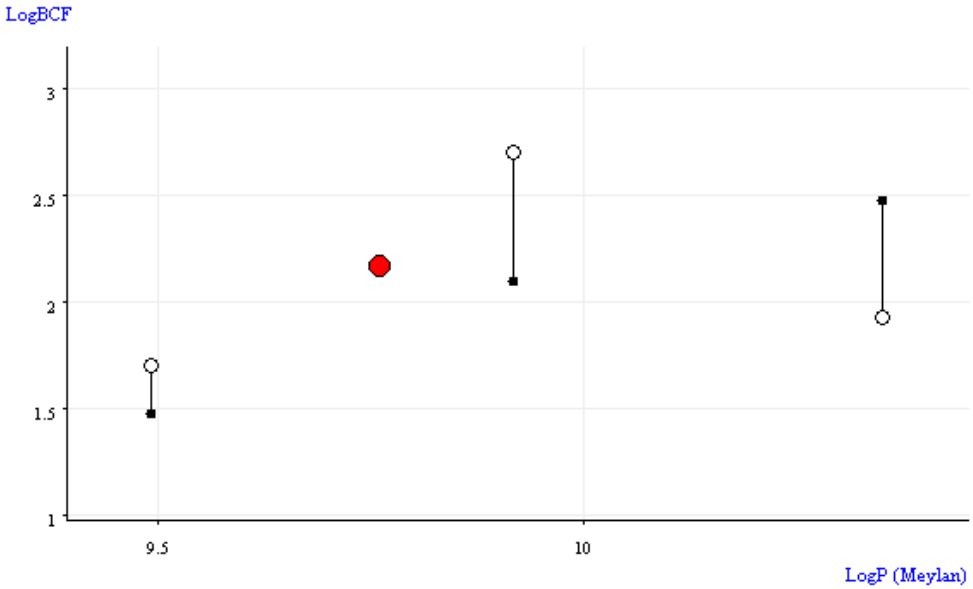
4.2 Reasoning:
Analysis of Molecular Descriptors

Descriptor name: LogP (Meylan)
Descriptor name: LogP is directly correlated to the logBCF value.

Following, a scatterplot of LogP (Meylan) against response values; experimental values are reported for the training set, predicted value for the studied compound. Light blue dots represent values of compounds from training set, red dot is the value of the studied compound.

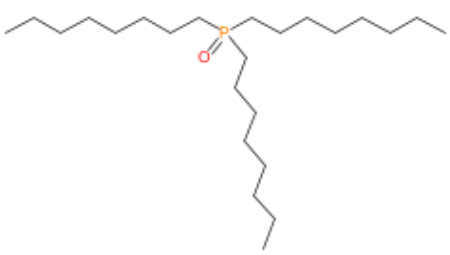


Following, a scatterplot of LogP (Meylan) against response values only for 3 most similar compounds in the training set. Red dot is the value of the studied compound, black outlined circles represents experimental values of compounds from training set, black dots represents predicted value of the same compound; the size of the circle is proportional to the similarity to the studied compound.



1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

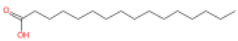
Prediction is 1.31 log(L/kg), but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- No similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not optimal
- some similar molecules found in the training set have experimental values that disagree with the predicted value
- the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability
- reliability of logP value used by the model is not optimal
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted BCF (up) [log(L/kg)]: 1.31
Predicted BCF (up) [L/kg]: 20
Predicted BCF (low) [log(L/kg)]: 1.49
Predicted BCF (low) [L/kg]: 31
Predicted BCF (mid) [log(L/kg)]: 1.45
Predicted BCF (mid) [L/kg]: 28
Predicted LogP (Meylan/Kowwin): 9.76
Predicted LogP reliability: Moderate
Predicted kM (Meylan): 1.82
Predicted kM reliability: Low
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 36653-82-4
Dataset id:728 (Training Set)
SMILES: OCCCCCCCCCCCCCCCC
Similarity: 0.729
Experimental value : 2.435
Predicted value : 2.771

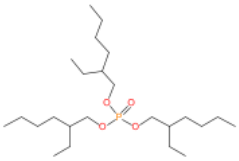


Compound #2

CAS: 57-10-3
Dataset id:705 (Training Set)
SMILES: O=C(O)CCCCCCCCCCCCCCC
Similarity: 0.726
Experimental value : 1.78
Predicted value : 2.918

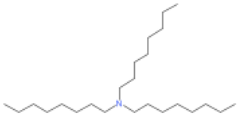
Compound #3

CAS: 10496-18-1
Dataset id:99 (Training Set)
SMILES: CCCCCCCCCCSSCCCCCCCCCC
Similarity: 0.721
Experimental value : 1.15
Predicted value : 0.516



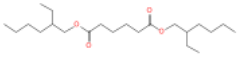
Compound #4

CAS: 78-42-2
Dataset id:199 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : 0.865
Predicted value : 0.087



Compound #5

CAS: 1116-76-3
Dataset id:72 (Training Set)
SMILES: N(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Similarity: 0.712
Experimental value : 1.86
Predicted value : 0.412



Compound #6

CAS: 103-23-1
Dataset id:195 (Training Set)
SMILES: O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Similarity: 0.697
Experimental value : 1.43
Predicted value : 0.698

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.291 Explanation: The predicted compound is outside the Applicability Domain of the model.
✖	Similar molecules with known experimental value Similarity index = 0.727 Explanation: No similar compounds with known experimental value in the training set have been found..
⚠	Accuracy of prediction for similar molecules Accuracy index = 0.737 Explanation: Accuracy of prediction for similar molecules found in the training set is not optimal..
⚠	Concordance for similar molecules Concordance index = 0.797 Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value..
✖	Maximum error of prediction among similar molecules Max error index = 1.138 Explanation: the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability..
⚠	Reliability of logP prediction LogP reliability = 0.7 Explanation: reliability of logP value used by the model is not optimal..
✖	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

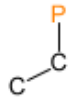
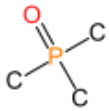
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

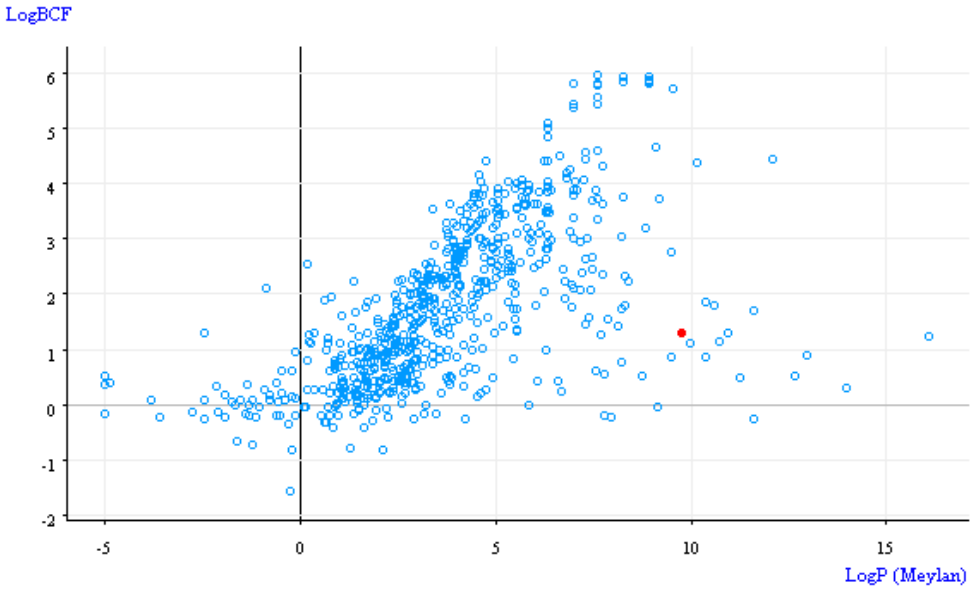
(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

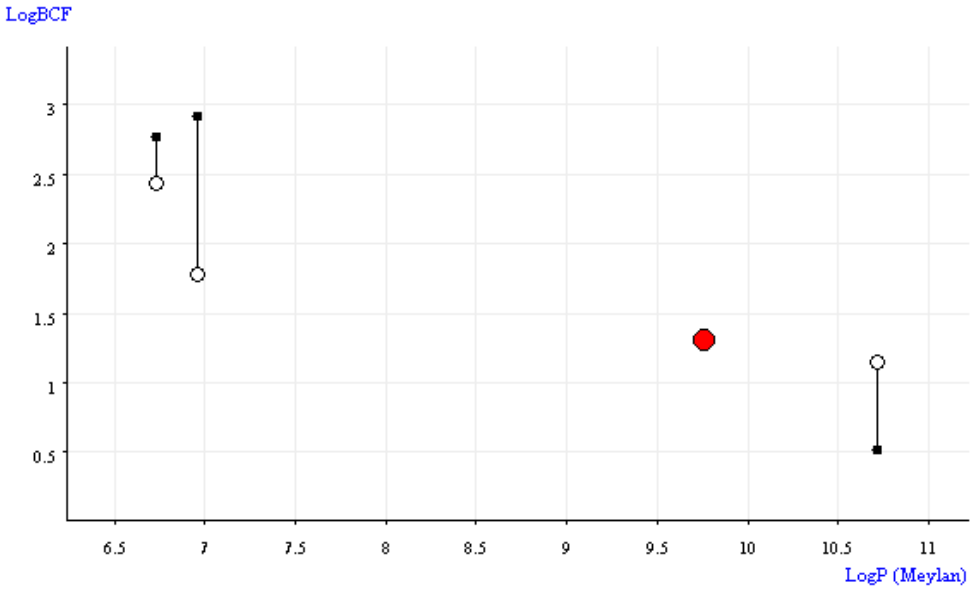
4.2 Reasoning:
Analysis of Molecular Descriptors

Descriptor name: LogP (Meylan)
Descriptor name: LogP is directly correlated to the logBCF value.

Following, a scatterplot of LogP (Meylan) against response values; experimental values are reported for the training set, predicted value for the studied compound. Light blue dots represent values of compounds from training set, red dot is the value of the studied compound.



Following, a scatterplot of LogP (Meylan) against response values only for 3 most similar compounds in the training set. Red dot is the value of the studied compound, black outlined circles represents experimental values of compounds from training set, black dots represents predicted value of the same compound; the size of the circle is proportional to the similarity to the studied compound.



1. Prediction Summary

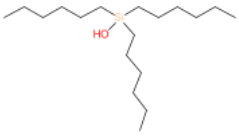
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is 1.91 log(L/kg), but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not optimal
- some similar molecules found in the training set have experimental values that disagree with the predicted value
- the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)

Compound: Molecule 0
Compound SMILES: O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Experimental value: -
Predicted BCF [log(L/kg)]: 1.91
Molecules used for prediction: 4
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

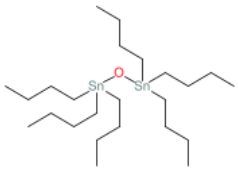


Compound #1

CAS: 60782-58-3
Dataset id:594 (Training Set)
SMILES: O[Si](CCCCCC)(CCCCCC)CCCCCC
Similarity: 0.726
Experimental value : 1.507
Predicted value : 2.973

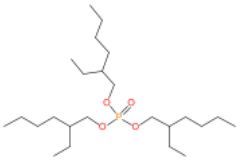
Compound #2

CAS: 10496-18-1
Dataset id:495 (Training Set)
SMILES: CCCCCCCCCCSSCCCCCCCCCC
Similarity: 0.721
Experimental value : 1.153
Predicted value : 0.52



Compound #3

CAS: 56-35-9
Dataset id:10 (Training Set)
SMILES: O([Sn](CCCC)(CCCC)CCCC)[Sn](CCCC)(CCCC)CCCC
Similarity: 0.715
Experimental value : 3.994
Predicted value : 2.815

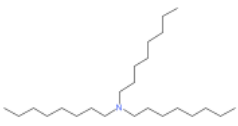


Compound #4

CAS: 78-42-2
Dataset id:49 (Training Set)
SMILES: O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Similarity: 0.714
Experimental value : 1.014
Predicted value : 1.183

Compound #5

CAS: 26787-65-5
Dataset id:539 (Training Set)
SMILES: O=C(OCCO)CCCCCCCCCCCCCCCCCCCCCCCCCC
Similarity: 0.713
Experimental value : 1.271
Predicted value : 1.278



Compound #6

CAS: 1116-76-3
Dataset id:402 (Training Set)
SMILES: N(CCCCCCCC)(CCCCCCCC)CCCCCCCC
Similarity: 0.712
Experimental value : 1.969
Predicted value : 0.739

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.288 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.719 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
⚠	Accuracy of prediction for similar molecules Accuracy index = 0.862 Explanation: Accuracy of prediction for similar molecules found in the training set is not optimal..
⚠	Concordance for similar molecules Concordance index = 1.034 Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value..
✖	Maximum error of prediction among similar molecules Max error index = 1.466 Explanation: the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability..
✖	Atom Centered Fragments similarity check ACF index = 0.4 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 unknown fragments found)..

Symbols explanation:

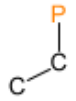
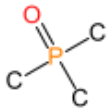
✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments .
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: CCP The fragment has never been found in the model's training set
	Fragment defined by the SMILES: CP(C)(C)=O The fragment has never been found in the model's training set

References and Documentation

You can find complete details on each model and on how to read results in the proper model's guide, available on-line at www.vega-qsar.eu or directly in the VegaNIC application.

Mutagenicity (Ames test) CONSENSUS model(version 1.0.4)

Mutagenicity (Ames test) Consensus model based on the predictions of VEGA mutagenicity models.

Mutagenicity (Ames test) model (CAESAR)(version 2.1.14)

QSAR classification model for Mutagenicity (from CAESAR project)

Mutagenicity (Ames test) model (ISS)(version 1.0.3)

Classification model for Mutagenicity (Ames test) based on Benigni-Bossa (Istituto Superiore di Sanità) rule set

Mutagenicity (Ames test) model (SarPy-IRFMN)(version 1.0.8)

QSAR classification model for Mutagenicity (SarPy/IRFMN)

References and Documentation

Mutagenicity (Ames test) model (KNN-Read-Across)(version 1.0.1)

KNN (Read-Across) model for Mutagenicity (Ames test)

Mutagenicity (Ames test) model for aromatic amines (CONCERT/IRFMN)(version 1.0.0)

A knowledge-based expert rule system for predicting mutagenicity (AMES test) of aromatic amines.

Carcinogenicity model (CAESAR)(version 2.1.10)

QSAR classification model for Carcinogenicity (from CAESAR project)

Carcinogenicity model (ISS)(version 1.0.3)

Classification model for Carcinogenicity based on Benigni-Bossa (Istituto Superiore di Sanità) rule set

References and Documentation

Carcinogenicity model (IRFMN-ISSCAN-CGX)(version 1.0.2)

QSAR classification model for Carcinogenicity (IRFMN/ISSCAN-CGX) based on the ISSCAN-CGX dataset

Carcinogenicity model (IRFMN-Antares)(version 1.0.2)

QSAR classification model for Carcinogenicity (IRFMN/Antares) based on the Antares dataset

Carcinogenicity oral classification model (IRFMN)(version 1.0.1)

Classification model for carcinogenicity (oral route).

Carcinogenicity oral Slope Factor model (IRFMN)(version 1.0.1)

Quantitative model for the carcinogenicity (oral route) Slope Factor.

References and Documentation

Carcinogenicity inhalation classification model (IRFMN)(version 1.0.1)

Classification model for carcinogenicity (inhalation route).

Carcinogenicity inhalation Slope Factor model (IRFMN)(version 1.0.1)

Quantitative model for the carcinogenicity inhalation route) Slope Factor.

Carcinogenicity in male rat (CORAL)(version 1.0.0)

Carcinogenicity in male rat quantitative (TD50) model model (CORAL)

Carcinogenicity in female Rat (CORAL)(version 1.0.0)

Carcinogenicity in female rat quantitative (TD50) model model (CORAL)

References and Documentation

Acute Toxicity (LD50) model (KNN)(version 1.0.0)

KNN model for acute toxicity (LD50)

BCF model (CAESAR)(version 2.1.15)

QSAR regression model for fish BCF (from CAESAR project)

BCF model (Meylan)(version 1.0.4)

QSAR regression model for fish BCF (based on Meylan model)

BCF model (Arnot-Gobas)(version 1.0.1)

QSAR regression model for fish BCF (based on Arnot-Gobas model)

References and Documentation

BCF model (KNN-Read-Across)(version 1.1.1)

KNN (Read-Across) model for fish BCF