CAESAR QSAR model for bioconcentration factor (BCF) in fish - version 1.0.0.11

The use of CAESAR models is regulated as in the license description available at the website.

More information on the CAESAR BCF model is available at the website.

http://www.caesar-project.eu

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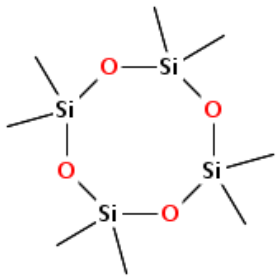
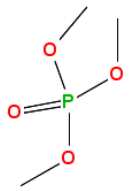
Prediction for the compound no. 1: C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1



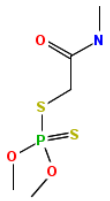
BCF value: 3 (L/Kg) whole body weight
Log BCF value: 0.47
Remarks for the prediction:
Presence of chemical features in the compound (Si atom in the molecule) that might be associated with a lower reliability of the predicted value.

The following chemicals similar to the query compound have been identified in the CAESAR database:



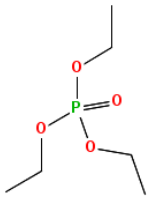
Dataset id: 406
SMILES: O=P(OC)(OC)OC
Similarity: 0.412

Experimental Log BCF: -0.52
Predicted Log BCF: 0.02



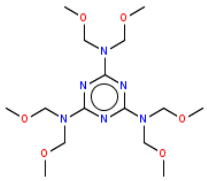
Dataset id: 464
SMILES: S=P(SCC(=O)NC)(OC)OC
Similarity: 0.404

Experimental Log BCF: -0.26
Predicted Log BCF: 0.09



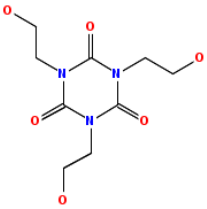
Dataset id: 404
SMILES: O=P(OCC)(OCC)OCC
Similarity: 0.386

Experimental Log BCF: -0.21
Predicted Log BCF: 0.58



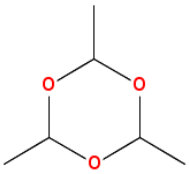
Dataset id: 442
SMILES: COCN(c1nc(nc(n1)N(COC)COC)N(COC)COC)COC
Similarity: 0.374

Experimental Log BCF: 0.28
Predicted Log BCF: 0.12



Dataset id: 444
SMILES: O=C1N(C(=O)N(C(=O)N1CCO)CCO)CCO
Similarity: 0.374

Experimental Log BCF: 0.20
Predicted Log BCF: 0.25



Dataset id: 462
SMILES: CC1OC(OC(O1)C)C
Similarity: 0.372

Experimental Log BCF: -0.52
Predicted Log BCF: 0.25

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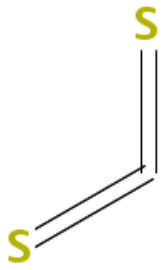
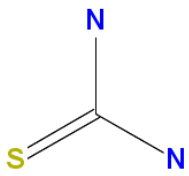
Prediction for the compound no. 2: S=C=S



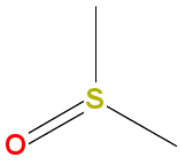
BCF value: 2 (L/Kg) whole body weight
Log BCF value: 0.24
Remarks for the prediction:
Descriptors for this compound have values outside the descriptor range for the compounds of the training set.

The following chemicals similar to the query compound have been identified in the CAESAR database:



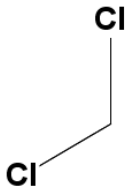
Dataset id: 399
SMILES: NC(=S)N
Similarity: 0.348

Experimental Log BCF: 0.30
Predicted Log BCF: 0.46



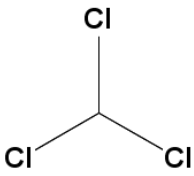
Dataset id: 398
SMILES: CS(=O)C
Similarity: 0.297

Experimental Log BCF: 0.60
Predicted Log BCF: 0.12



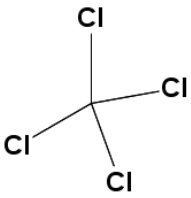
Dataset id: 240
SMILES: ClCCl
Similarity: 0.29

Experimental Log BCF: 1.37
Predicted Log BCF: 0.57



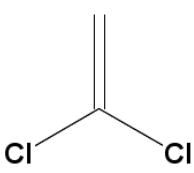
Dataset id: 241
SMILES: ClC(Cl)Cl
Similarity: 0.286

Experimental Log BCF: 0.93
Predicted Log BCF: 0.61



Dataset id: 242
SMILES: ClC(Cl)(Cl)Cl
Similarity: 0.283

Experimental Log BCF: 0.87
Predicted Log BCF: 0.61



Dataset id: 259
SMILES: C=C(Cl)Cl
Similarity: 0.279

Experimental Log BCF: 0.95
Predicted Log BCF: 0.51