

3,3,3-Trifluoro-2,2-bis(trifluoromethyl)propanoic acid
917951-63-4 | DTXSID00633413

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.10 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.73e-01

Confidence level: 2.83e-01

Nearest Neighbors from the Training Set

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1-Butanol, 2,2,3,3,4,4,4-heptafluoro-

Measured: 6.37

Predicted: 42.6

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2-Methyl-2-butanol

Measured: 110

Predicted: 9.41

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1-Decene

Measured: 159

Predicted: 1.31

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Ethane, 1,1-dichloro-1,2,2,2-tetrafluoro-

Measured: 33.1

Predicted: 2170

Image not found

Fenamiphos

Measured: 3.00e-04

Predicted: 1.06e-06