

Acetic acid, trifluoro-, methyl ester
431-47-0 | DTXSID2059988

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: 369 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.46e-01

Confidence level: 7.87e-01

Nearest Neighbors from the Training Set

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Butamiphos

Measured: 236

Predicted: 8.98e-05

[Image not found](#)

2,3',4',5-Tetrachlorobiphenyl

Measured: 227

Predicted: 2.94e-05

[Image not found](#)

Buprofezin

Measured: 370

Predicted: 4.96e-06

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Cyclopropane carboxylic acid

Measured: 645

Predicted: 2.37e-01

[Image not found](#)

Methoxyethene

Measured: 586

Predicted: 814