

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.30e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.19e-01

Confidence level: 5.24e-01

Nearest Neighbors from the Training Set

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Ethyl 4,4,4-trifluoroacetoacetate

Measured: 4.35e-02

Predicted: 7.99e-02

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Sarin

Measured: 7.14

Predicted: 1.65

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Diisopropyl fluorophosphate

Measured: 8.36e-02

Predicted: 8.23e-02

Image not found

Dimefox

Measured: 6.49

Predicted: 4.15

Image not found

Mipafos

Measured: 4.39e-01

Predicted: 4.12e-01