

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 43.4 °C

Global applicability domain: Inside

Local applicability domain index: 6.11e-01

Confidence level: 8.37e-01

Nearest Neighbors from the Training Set

Image not found

Acetic acid, trifluoro-, methyl ester

Measured: 43.3

Predicted: 43.4

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2-Propanone, 1,1,1-trifluoro-

Measured: 22.0

Predicted: 26.6

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Ethane, 1-ethoxy-1,1,2,2-tetrafluoro-

Measured: 57.5

Predicted: 54.1

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Ethyl trifluoroacetate

Measured: 61.0

Predicted: 60.5

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Ethene, (2,2,2-trifluoroethoxy)-

Measured: 42.5

Predicted: 45.8