

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 7.19e-01

Global applicability domain: Inside

Local applicability domain index: 5.59e-01

Confidence level: 7.77e-01

Nearest Neighbors from the Training Set

Image not found

Acetic acid, trifluoro-, methyl ester

Measured: 0.6

Predicted: 7.19e-01

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Ethyl trifluoroacetate

Measured: 1.18

Predicted: 1.04

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1-Propanol, 2,2,3,3,3-pentafluoro-

Measured: 1.23

Predicted: 1.14

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Acetic acid, difluoro-, ethyl ester

Measured: 0.87

Predicted: 8.28e-01

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2,2,2-trifluoro-N-methylethanamine

Measured: 0.55

Predicted: 5.98e-01