

Acetic acid, trifluoro-
76-05-1 | DTXSID9041578

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: 6.47e-01

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 7.86e-01

Nearest Neighbors from the Training Set

Image not found

2,2,2-Trifluoroethanol

Measured: 0.41

Predicted: 3.51e-01

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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Acetic acid, difluoro-, ethyl ester

Measured: 0.87

Predicted: 8.28e-01

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Ethanamine, 2,2,2-trifluoro-

Measured: 0.24

Predicted: 3.15e-01