

2,2,2-Trifluoroethanol
75-89-8 | DTXSID0021751

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 2.68

Global applicability domain: Inside

Local applicability domain index: 9.07e-01

Confidence level: 5.72e-01

Nearest Neighbors from the Training Set

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Methanol

Measured: 2.88

Predicted: 2.66

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Methylamine

Measured: 1.90

Predicted: 2.59

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Dimethylamine

Measured: 2.00

Predicted: 2.62

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Ethanol

Measured: 3.25

Predicted: 3.05

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Acetic acid

Measured: 4.31

Predicted: 3.69