

Trifluoromethanesulfonic acid
1493-13-6 | DTXSID2044397

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 18.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.64e-01

Confidence level: 6.34e-01

Nearest Neighbors from the Training Set

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Trichloroacetic acid

Measured: 2.00

Predicted: 3.40

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Chloropicrin

Measured: 61.7

Predicted: 61.7

Image not found

Chloroform

Measured: 39.8

Predicted: 50.3

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2,2,2-Trichloroacetamide

Measured: 9.77

Predicted: 6.26

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Trichloroethylene

Measured: 100

Predicted: 83.1