

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.67e-15 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.58e-01

Confidence level: 5.76e-01

Nearest Neighbors from the Training Set

Image not found

1,2-Dibromo-1,1,2,2-tetrafluoroethane

Measured: 1.30e-16

Predicted: 2.57e-16

Image not found

1,1,1,2,3,3,3-heptafluoropropane

Measured: 1.62e-15

Predicted: 2.76e-15

Image not found

Perfluorotriethylamine

Measured: 6.00e-16

Predicted: 6.45e-16

Image not found

3,3-dichloro-1,1,1,2,2-pentafluoropropane

Measured: 2.50e-14

Predicted: 1.18e-14