

1,1,2,2-Tetrafluoro-2-(1,2,2,2-tetrafluoroethoxy)ethane-1-sulfonyl fluoride
446312-61-4 | DTXSID00580271

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: 2.69

Global applicability domain: Inside

Local applicability domain index: 9.94e-01

Confidence level: 6.36e-01

Nearest Neighbors from the Training Set

Image not found

1-Nitropropane

Measured: 3.25

Predicted: 2.53

Image not found

Chloroform

Measured: 2.80

Predicted: 2.69

Image not found

Methyl tert-butyl ether

Measured: 2.58

Predicted: 2.53

Image not found

Pentane

Measured: 1.96

Predicted: 2.68

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2-Methylpropanenitrile

Measured: 2.87

Predicted: 2.60