

Perfluorotributylamine
311-89-7 | DTXSID0027141

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.41e-04 mol/L

Global applicability domain: Outside

Local applicability domain index: 1.42e-01

Confidence level: 6.32e-01

Nearest Neighbors from the Training Set

Image not found

Chloropentafluoroethane

Measured: 3.82e-04

Predicted: 7.63e-04

Image not found

Dithiopyr

Measured: 3.49e-06

Predicted: 6.15e-05

Image not found

Thiazopyr

Measured: 6.31e-06

Predicted: 2.84e-05

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Ethane, 1,1-dichloro-1,2,2,2-tetrafluoro-

Measured: 8.01e-04

Predicted: 1.41e-03

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2-Chloro-1,1,1,2-tetrafluoroethane

Measured: 1.10e-02

Predicted: 8.36e-03