

Perfluorotriethylamine
359-70-6 | DTXSID40189464

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 69.2 °C

Global applicability domain: Outside

Local applicability domain index: 2.85e-01

Confidence level: 8.91e-01

Nearest Neighbors from the Training Set

Image not found

Perfluorotriethylamine

Measured: 70.3

Predicted: 69.2

Image not found

Morpholine, 2,2,3,3,5,5,6,6-octafluoro-4-(trifluoromethyl)-

Measured: 51.0

Predicted: 52.0

Image not found

Perfluoroheptane

Measured: 82.5

Predicted: 78.8

Image not found

Perflexane

Measured: 56.6

Predicted: 57.0

Image not found

1,1,1,2,2,3,4,4,5,5,5-Undecafluoro-3-(trifluoromethyl)pentane

Measured: 58.4

Predicted: 57.8