

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 178 °C

Global applicability domain: Outside

Local applicability domain index: 2.80e-01

Confidence level: 7.69e-01

Nearest Neighbors from the Training Set

Image not found

Perfluorotributylamine

Measured: 178

Predicted: 178

Image not found

1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6-[(tridecafluorohexyl)oxy]hexane

Measured: 181

Predicted: 183

Image not found

1-Propanamine, 1,1,2,2,3,3,3-heptafluoro-N,N-bis(heptafluoropropyl)-

Measured: 130

Predicted: 129

Image not found

Perflubrodec

Measured: 198

Predicted: 194

Image not found

Tetracosafuorotetradecahydrophenanthrene

Measured: 210

Predicted: 206