

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1740

Global applicability domain: Outside

Local applicability domain index: 1.51e-01

Confidence level: 4.90e-01

Nearest Neighbors from the Training Set

Image not found

1,1'-Isopropylidenebis(4-(1,1,2,2-tetrafluoroethoxy)benzene)

Measured: 22400

Predicted: 356

Image not found

2,2,4,4,6,8,8-Heptamethylnonane

Measured: 6610

Predicted: 6010

Image not found

Tris(2,3-dibromopropyl)phosphate

Measured: 3.24

Predicted: 5.93

Image not found

1,3,5-Tri-tert-butylbenzene

Measured: 22900

Predicted: 3970

Image not found

2,2,4,6,6-Pentamethylheptane

Measured: 871

Predicted: 963