

1,5,7,11-Tetraoxaspiro[5.5]undecane
24472-02-4 | DTXSID1066994

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 60.6 °C

Global applicability domain: Inside

Local applicability domain index: 4.32e-01

Confidence level: 3.41e-01

Nearest Neighbors from the Training Set

Image not found

2,4,8,10-

Tetraoxaspiro[5.5]undecane

Measured: 48.3

Predicted: 59.0

Image not found

Paraldehyde

Measured: 12.6

Predicted: 16.3

Image not found

2,3-DIMETHOXY-5,6-DIMETHYL-
P-BENZOQUINONE

Measured: 62.5

Predicted: 86.4

Image not found

Ubiquinone-O

Measured: 59.5

Predicted: 97.6