

Isopropanol-d7
19214-96-1 | DTXSID50480717

Model Performance

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

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: 4.07

Global applicability domain: Inside

Local applicability domain index: 5.27e-01

Confidence level: 8.46e-01

Nearest Neighbors from the Training Set

[Image not found](#)

tert-Butyl alcohol

Measured: 5.01

Predicted: 4.48

[Image not found](#)

Dimethyl sulfoxide

Measured: 3.98

Predicted: 4.07

[Image not found](#)

Diethyl ether

Measured: 5.37

Predicted: 4.72

[Image not found](#)

3-Pyridinamine

Measured: 2.09

Predicted: 3.04

[Image not found](#)

4-Aminopyridine

Measured: 4.57

Predicted: 3.04