

Ethane, methoxy-d3
16995-14-5 | DTXSID20168777

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: 14.4 °C

Global applicability domain: Inside

Local applicability domain index: 6.80e-01

Confidence level: 7.80e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl methyl ether

Measured: 7.40

Predicted: 14.4

Image not found

2-Chloropropane

Measured: 35.7

Predicted: 33.9

Image not found

1-Chloropropane

Measured: 46.5

Predicted: 43.0

Image not found

Butane

Measured: -0.500

Predicted: 5.22

Image not found

Peroxide, dimethyl

Measured: 14.0

Predicted: 18.4