

Propane
74-98-6 | DTXSID5026386

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -160 °C

Global applicability domain: Inside

Local applicability domain index: 8.68e-01

Confidence level: 5.62e-01

Nearest Neighbors from the Training Set

Image not found

Propane

Measured: -188

Predicted: -160

Image not found

Butane

Measured: -138

Predicted: -147

Image not found

Isobutane

Measured: -138

Predicted: -122

Image not found

Pentane

Measured: -130

Predicted: -136

Image not found

2-Methylbutane

Measured: -160

Predicted: -119