

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: -29.2 °C

Global applicability domain: Inside

Local applicability domain index: 6.55e-01

Confidence level: 4.17e-01

Nearest Neighbors from the Training Set

Image not found

Propane

Measured: -42.1

Predicted: -29.2

Image not found

Dimethyl ether

Measured: -24.8

Predicted: -26.1

Image not found

Chloroethane

Measured: 12.3

Predicted: 8.50

Image not found

Dimethylboranyl

Measured: 70.5

Predicted: 27.2

Image not found

Ethylene

Measured: -104

Predicted: -71.5