

Nonane

111-84-2 | DTXSID9025796

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: -37.0 °C

Global applicability domain: Inside

Local applicability domain index: 9.75e-01

Confidence level: 8.25e-01

Nearest Neighbors from the Training Set

Image not found

Nonane

Measured: -53.5

Predicted: -37.0

Image not found

Decane

Measured: -29.7

Predicted: -25.8

Image not found

Octane

Measured: -56.8

Predicted: -68.5

Image not found

Undecane

Measured: -25.6

Predicted: -14.0

Image not found

Dodecane

Measured: -9.60

Predicted: -12.6