

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: -68.5 °C

Global applicability domain: Inside

Local applicability domain index: 9.68e-01

Confidence level: 7.84e-01

Nearest Neighbors from the Training Set

Image not found

Octane

Measured: -56.8

Predicted: -68.5

Image not found

Nonane

Measured: -53.5

Predicted: -37.0

Image not found

Heptane

Measured: -90.6

Predicted: -94.2

Image not found

Decane

Measured: -29.7

Predicted: -25.8

Image not found

4-Methylheptane

Measured: -121

Predicted: -110