

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: -73.5 °C

Global applicability domain: Inside

Local applicability domain index: 9.52e-01

Confidence level: 6.14e-01

Nearest Neighbors from the Training Set

Image not found

Cumene

Measured: -96.0

Predicted: -73.5

Image not found

p-Isopropyl-alpha-methylstyrene

Measured: -30.6

Predicted: -62.9

Image not found

sec-Butylbenzene

Measured: -82.7

Predicted: -76.5

Image not found

3-Ethyltoluene

Measured: -95.5

Predicted: -70.4

Image not found

4-Ethyltoluene

Measured: -62.3

Predicted: -70.4