

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: 216 °C

Global applicability domain: Inside

Local applicability domain index: 7.10e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

Image not found

Dodecane

Measured: 216

Predicted: 216

Image not found

1-Dodecene

Measured: 214

Predicted: 215

Image not found

5-Butylnonane

Measured: 218

Predicted: 222

Image not found

Tridecane

Measured: 235

Predicted: 231

Image not found

Undecane

Measured: 196

Predicted: 192