

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: 296 °C

Global applicability domain: Inside

Local applicability domain index: 2.58e-01

Confidence level: 6.76e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Chloramben

Measured: 312

Predicted: 301

[Image not found](#)

2-Aminobenzamide

Measured: 300

Predicted: 299

[Image not found](#)

4-Aminoacetanilide

Measured: 267

Predicted: 290

[Image not found](#)

2-Nitrobenzamide

Measured: 317

Predicted: 310