

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: 183 °C

Global applicability domain: Inside

Local applicability domain index: 3.70e-01

Confidence level: 4.88e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Sulfanilamide

Measured: 166

Predicted: 164

[Image not found](#)

4-Amino-3,5-dichlorobenzoic acid

Measured: 292

Predicted: 241

[Image not found](#)

Chloramben

Measured: 200

Predicted: 211

[Image not found](#)

Benzenesulfonyl hydrazide

Measured: 102

Predicted: 114