

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: 291 °C

Global applicability domain: Inside

Local applicability domain index: 5.61e-01

Confidence level: 8.22e-01

Nearest Neighbors from the Training Set

[Image not found](#)

MCPA

Measured: 287

Predicted: 278

[Image not found](#)

Mecoprop

Measured: 298

Predicted: 282

[Image not found](#)

1-Naphthalenecarboxylic acid,
3,4-dihydro-

Measured: 306

Predicted: 300

[Image not found](#)

2,5-Dichlorobenzoic acid

Measured: 301

Predicted: 288