

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: 399 °C

Global applicability domain: Inside

Local applicability domain index: 2.80e-01

Confidence level: 4.46e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Alizarin

Measured: 430

Predicted: 399

[Image not found](#)

(1,1'-Biphenyl)-2,2'-diol

Measured: 320

Predicted: 315

[Image not found](#)

2,2'-Dihydroxybenzophenone

Measured: 333

Predicted: 318

[Image not found](#)

Hexachlorophene

Measured: 479

Predicted: 416

[Image not found](#)

Benzenemethanol,
.alpha.,.alpha.-diphenyl-

Measured: 380

Predicted: 348