

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: 128 °C

Global applicability domain: Inside

Local applicability domain index: 7.73e-01

Confidence level: 6.02e-01

Nearest Neighbors from the Training Set

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Resorcinol

Measured: 111

Predicted: 128

[Image not found](#)

Hydroquinone

Measured: 172

Predicted: 138

[Image not found](#)

1,3-Benzenediol, 5-methyl-

Measured: 108

Predicted: 111

[Image not found](#)

1,3-Benzenediol, 4-methyl-

Measured: 106

Predicted: 111

[Image not found](#)

4-Hydroxybenzenemethanol

Measured: 125

Predicted: 101