

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: 133 °C

Global applicability domain: Inside

Local applicability domain index: 9.12e-01

Confidence level: 3.89e-01

Nearest Neighbors from the Training Set

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1,2-Diphenoxyethane

Measured: 98.0

Predicted: 127

[Image not found](#)

2,2'-Dimethoxybiphenyl

Measured: 155

Predicted: 128

[Image not found](#)

3,3'-Dimethoxy-1,1'-biphenyl

Measured: 36.0

Predicted: 127

[Image not found](#)

1,1'-Biphenyl, 4,4'-dimethoxy-

Measured: 175

Predicted: 128