

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: 214 °C

Global applicability domain: Inside

Local applicability domain index: 9.72e-01

Confidence level: 8.89e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Menthol

Measured: 212

Predicted: 214

[Image not found](#)

Cyclohexanol, 1-methyl-4-(1-methylethyl)-

Measured: 209

Predicted: 214

[Image not found](#)

Citronellol

Measured: 224

Predicted: 223

[Image not found](#)

Citronellol

Measured: 224

Predicted: 223