

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: 39.2 °C

Global applicability domain: Inside

Local applicability domain index: 8.60e-01

Confidence level: 8.28e-01

Nearest Neighbors from the Training Set

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Menthol

Measured: 39.0

Predicted: 39.2

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2-tert-Butylcyclohexanol

Measured: 45.0

Predicted: 39.4

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1-Ethylcyclohexanol

Measured: 34.5

Predicted: 41.7

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beta-Terpineol

Measured: 32.5

Predicted: 45.2

Image not found

alpha-Terpineol

Measured: 37.0

Predicted: 42.3

Image not found

alpha-Terpineol

Measured: 37.0

Predicted: 42.3

Image not found

alpha-Terpineol

Measured: 37.0

Predicted: 42.3

