

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: 233 °C

Global applicability domain: Inside

Local applicability domain index: 4.35e-01

Confidence level: 5.75e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethyl N-butylcarbamate

Measured: 202

Predicted: 193

[Image not found](#)

Dodecanenitrile

Measured: 277

Predicted: 269

[Image not found](#)

Isovaleryl diethylamide

Measured: 211

Predicted: 210

[Image not found](#)

Tridecanenitrile

Measured: 293

Predicted: 282