

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:** 237 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 4.49e-01

**Confidence level:** 6.02e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Ethyl N-butylcarbamate

**Measured:** 202

**Predicted:** 193

[Image not found](#)

4-benzylmorpholine

**Measured:** 261

**Predicted:** 254

[Image not found](#)

1-Benzylpiperidine

**Measured:** 245

**Predicted:** 251

[Image not found](#)

N,N-Dimethyl-p-bromoaniline

**Measured:** 264

**Predicted:** 245