

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:** 352 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 5.09e-01

**Confidence level:** 5.90e-01

## Nearest Neighbors from the Training Set

Image not found

3,3'-Dimethylbenzidine

**Measured:** 339

**Predicted:** 371

Image not found

4,4'-Thiodianiline

**Measured:** 361

**Predicted:** 359

Image not found

1,2-Benzenediamine,N-phenyl-

**Measured:** 313

**Predicted:** 363

Image not found

N-Phenyl-1,4-benzenediamine

**Measured:** 354

**Predicted:** 363

Image not found

4,4'-Methylenedianiline

**Measured:** 398

**Predicted:** 368