

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:** 117 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 7.17e-01

**Confidence level:** 7.39e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Morpholine

**Measured:** 128

**Predicted:** 117

[Image not found](#)

Piperidine

**Measured:** 106

**Predicted:** 113

[Image not found](#)

Cyclopentanamine

**Measured:** 108

**Predicted:** 114

[Image not found](#)

Pyrrolidine

**Measured:** 86.5

**Predicted:** 90.2

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Pyridine, 1,2,3,6-tetrahydro-

**Measured:** 108

**Predicted:** 112