

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

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: 47.1 °C

Global applicability domain: Inside

Local applicability domain index: 7.12e-01

Confidence level: 8.16e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Propanal

Measured: 48.0

Predicted: 47.1

[Image not found](#)

Acetone

Measured: 55.8

Predicted: 48.2

[Image not found](#)

(2H6)Acetone

Measured: 55.8

Predicted: 50.0

[Image not found](#)

Methyl formate

Measured: 31.7

Predicted: 36.7

[Image not found](#)

1,3-Propylene oxide

Measured: 47.6

Predicted: 40.7