

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: 271 °C

Global applicability domain: Inside

Local applicability domain index: 6.47e-01

Confidence level: 7.28e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Resorcinol

Measured: 280

Predicted: 271

[Image not found](#)

Hydroquinone

Measured: 287

Predicted: 271

[Image not found](#)

4-Hydroxybenzenemethanol

Measured: 252

Predicted: 275

[Image not found](#)

Catechol

Measured: 246

Predicted: 263

[Image not found](#)

1,3-Benzenediol, 5-methyl-

Measured: 290

Predicted: 269