

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.84 | 0.55 | 0.85 | 0.53 | 0.83 | 0.64 |

Model Results

Predicted value: 45.7

Global applicability domain: Inside

Local applicability domain index: 5.11e-01

Confidence level: 5.75e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isoamyl ether

Measured: 170

Predicted: 137

[Image not found](#)

Molinate

Measured: 25.7

Predicted: 14.8

[Image not found](#)

1-Ethenoxy-2-ethylhexane

Measured: 603

Predicted: 284

[Image not found](#)

Tributylamine

Measured: 25.1

Predicted: 23.2