

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: 30.9 °C

Global applicability domain: Inside

Local applicability domain index: 3.37e-01

Confidence level: 5.12e-01

Nearest Neighbors from the Training Set

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Malathion

Measured: 2.80

Predicted: 7.96

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Formothion

Measured: 25.5

Predicted: 29.7

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cis-Mevinphos

Measured: 21.0

Predicted: 15.8

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Phenthoate

Measured: 17.5

Predicted: 9.82