

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 3.41

Global applicability domain: Inside

Local applicability domain index: 7.21e-01

Confidence level: 7.94e-01

Nearest Neighbors from the Training Set

Image not found

EPTC

Measured: 3.21

Predicted: 3.41

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Pebulate

Measured: 3.83

Predicted: 3.70

Image not found

Vernolate

Measured: 3.84

Predicted: 3.79

Image not found

Molinate

Measured: 3.21

Predicted: 3.26

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Cycloate

Measured: 3.88

Predicted: 3.94