

Model Performance

Model	Data
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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: 3.94

Global applicability domain: Inside

Local applicability domain index: 6.26e-01

Confidence level: 6.61e-01

Nearest Neighbors from the Training Set

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Cycloate

Measured: 3.88

Predicted: 3.94

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Vernolate

Measured: 3.84

Predicted: 3.79

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Butylate

Measured: 4.15

Predicted: 4.00

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Pebulate

Measured: 3.83

Predicted: 3.70

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Diallate

Measured: 4.49

Predicted: 4.18