

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.22

Global applicability domain: Inside

Local applicability domain index: 2.92e-01

Confidence level: 7.44e-01

Nearest Neighbors from the Training Set

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Triisopropanolamine

Measured: 5.75e-01

Predicted: 7.42e-01

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Hexamethylphosphoramide

Measured: 5.01e-01

Predicted: 7.23e-01

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Pentaerythritol

Measured: 1.26

Predicted: 1.25

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Triethanolamine

Measured: 3.89

Predicted: 2.97

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Cycloheximide

Measured: 2.82

Predicted: 2.70