

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: 1.43

Global applicability domain: Inside

Local applicability domain index: 4.07e-01

Confidence level: 7.63e-01

Nearest Neighbors from the Training Set

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Triethyl phosphate

Measured: 1.29

Predicted: 1.38

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Trimethyl phosphate

Measured: 1.41

Predicted: 1.50

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Triallyl phosphate

Measured: 1.20

Predicted: 1.41

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2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00

Predicted: 1.47

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Paraldehyde

Measured: 3.02

Predicted: 2.77