

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: 8.29

Global applicability domain: Inside

Local applicability domain index: 5.70e-01

Confidence level: 8.44e-01

Nearest Neighbors from the Training Set

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2-Nitropropane

Measured: 8.32

Predicted: 7.41

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Furan

Measured: 5.01

Predicted: 4.88

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Carbon disulfide

Measured: 19.5

Predicted: 17.4

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Thiophene

Measured: 8.91

Predicted: 6.68

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Diethyl ether

Measured: 5.37

Predicted: 4.72