

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: 3.39

Global applicability domain: Inside

Local applicability domain index: 5.28e-01

Confidence level: 6.38e-01

Nearest Neighbors from the Training Set

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1-Methoxynaphthalene

Measured: 3.45

Predicted: 2.91

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Precocene I

Measured: 3.35

Predicted: 3.02

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1,2-Diphenoxyethane

Measured: 3.81

Predicted: 3.37

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2-Methoxynaphthalene

Measured: 3.47

Predicted: 2.55