

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.33

Global applicability domain: Inside

Local applicability domain index: 9.56e-01

Confidence level: 5.88e-01

Nearest Neighbors from the Training Set

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Piperidine

Measured: 4.04

Predicted: 4.32

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1-Pentanol

Measured: 4.69

Predicted: 4.17

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Dipropylamine

Measured: 3.59

Predicted: 4.37

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Isopentyl alcohol

Measured: 4.52

Predicted: 4.24

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1-Hexanol

Measured: 5.18

Predicted: 4.67