

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: 8.63

Global applicability domain: Inside

Local applicability domain index: 6.90e-01

Confidence level: 3.72e-01

Nearest Neighbors from the Training Set

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Phenacetin

Measured: 9.59

Predicted: 9.23

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Diphenylamine

Measured: 7.64

Predicted: 8.73

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Methylparaben

Measured: 8.57

Predicted: 7.06

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1-Hexadecanol

Measured: 9.90

Predicted: 9.79

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1-Octanol

Measured: 6.03

Predicted: 5.95