

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: 2.65e-01

Global applicability domain: Inside

Local applicability domain index: 6.20e-01

Confidence level: 6.32e-01

Nearest Neighbors from the Training Set

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Butyraldehyde

Measured: 0.88

Predicted: 7.87e-01

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2-Chloroethanol

Measured: 0.03

Predicted: -0.00475

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Fluoroacetone

Measured: -0.390

Predicted: 1.41e-01

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Propanal

Measured: 0.59

Predicted: 5.24e-01

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Allyl alcohol

Measured: 0.17

Predicted: 9.34e-02