

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: 2.11

Global applicability domain: Inside

Local applicability domain index: 9.85e-01

Confidence level: 7.16e-01

Nearest Neighbors from the Training Set

Image not found

Butane

Measured: 1.53

Predicted: 2.22

Image not found

Dichloromethane

Measured: 2.27

Predicted: 2.41

Image not found

Methyl acetate

Measured: 2.31

Predicted: 2.41

Image not found

Ethyl formate

Measured: 2.19

Predicted: 2.41

Image not found

Acetone

Measured: 2.31

Predicted: 2.42