

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: 5.24e-01

Global applicability domain: Inside

Local applicability domain index: 6.30e-01

Confidence level: 6.99e-01

Nearest Neighbors from the Training Set

Image not found

Propanal

Measured: 0.59

Predicted: 5.24e-01

Image not found

Butyraldehyde

Measured: 0.88

Predicted: 7.87e-01

Image not found

Vinyl acetate

Measured: 0.73

Predicted: 8.06e-01

Image not found

Acetone

Measured: -0.240

Predicted: 3.35e-02

Image not found

Allyl alcohol

Measured: 0.17

Predicted: 9.34e-02