

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.23e-08 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.06e-01

Confidence level: 5.08e-01

Nearest Neighbors from the Training Set

Image not found

Tridecane

Measured: 2.55e-08

Predicted: 1.55e-08

Image not found

Undecane

Measured: 2.82e-08

Predicted: 1.58e-07

Image not found

Tetradecane

Measured: 1.97e-08

Predicted: 1.05e-08

Image not found

Decane

Measured: 3.65e-07

Predicted: 4.95e-07

Image not found

Octane, 4,4-dimethyl-

Measured: 1.55e-05

Predicted: 6.33e-06