

Model Performance

Model	Data
-------	------

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: 1.73e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.54e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

Image not found

4-(1-Naphthyl)-4-oxobutanoic acid

Measured: 3.29e-04

Predicted: 3.91e-03

Image not found

4-(2-Naphthyl)-4-oxobutanoic acid

Measured: 1.40e-04

Predicted: 3.91e-03

Image not found

3,5-Dibromo-2-hydroxycyclohepta-2,4,6-trien-1-one

Measured: 3.14e-04

Predicted: 6.20e-04

Image not found

1-Naphthalenecarboxylic acid, 8-nitro-

Measured: 1.78e-03

Predicted: 2.02e-02