

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 10.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.44e-01

Confidence level: 5.78e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Dioxane

Measured: 17.0

Predicted: 13.2

Image not found

2,2'-Bioxirane

Measured: 2.51

Predicted: 4.97

Image not found

1,2-Propylene glycol

Measured: 2.29

Predicted: 4.24

Image not found

Acrylamide

Measured: 50.1

Predicted: 16.7

Image not found

Pyridine

Measured: 39.8

Predicted: 20.1