

Model Performance

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

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: 4.45 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.15e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

Image not found

1-Propanol

Measured: 3.02

Predicted: 4.69

Image not found

Ethanol

Measured: 1.58

Predicted: 2.24

Image not found

1-Butanol

Measured: 3.16

Predicted: 8.95

Image not found

Thioacetamide

Measured: 6.03

Predicted: 6.43

Image not found

Pyridine

Measured: 39.8

Predicted: 20.1