

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: 116 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.64e-01

Confidence level: 8.40e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4,4'-Methylenedianiline

Measured: 97.7

Predicted: 87.8

[Image not found](#)

4,4'-Thiodianiline

Measured: 110

Predicted: 116

[Image not found](#)

Ethyl 1-naphthaleneacetate

Measured: 302

Predicted: 425

[Image not found](#)

N-(1,1-dimethyl-2-propynyl)-4-methoxybenzamide

Measured: 67.6

Predicted: 72.5

[Image not found](#)

N-Cyclopentyl-N'-phenylurea

Measured: 85.1

Predicted: 122