

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:** 17.8 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 5.34e-01

**Confidence level:** 8.22e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Dalapon

**Measured:** 2.51

**Predicted:** 2.04

[Image not found](#)

Dalapon-sodium

**Measured:** 1.00

**Predicted:** 2.04

[Image not found](#)

2,4-Dichloroaniline

**Measured:** 525

**Predicted:** 465

[Image not found](#)

4-Bromo-m-toluidine

**Measured:** 182

**Predicted:** 173

[Image not found](#)

2-Chlorobenzamide

**Measured:** 32.4

**Predicted:** 37.2