

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:** 51.7 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 3.35e-01

**Confidence level:** 7.53e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Diethylacetamide

**Measured:** 69.2

**Predicted:** 64.5

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Allidochlor

**Measured:** 20.0

**Predicted:** 24.7

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Benzamide, N,N-dimethyl-

**Measured:** 39.8

**Predicted:** 36.3

[Image not found](#)

Dichlormid

**Measured:** 39.8

**Predicted:** 46.7

[Image not found](#)

N,N-Dimethylaniline

**Measured:** 182

**Predicted:** 130