

1-Chloro-1-nitropropane
600-25-9 | DTXSID2024797

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: 63.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.18e-01

Confidence level: 6.45e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Chlorobenzene

Measured: 141

Predicted: 106

[Image not found](#)

3-Chlorophenol

Measured: 347

Predicted: 108

[Image not found](#)

Resorcinol

Measured: 9.55

Predicted: 28.3

[Image not found](#)

1,2-Dichloropropane

Measured: 46.8

Predicted: 48.0

[Image not found](#)

Phenol

Measured: 26.9

Predicted: 57.3