

Benzonitrile
100-47-0 | DTXSID7021491

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: 53.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.76e-01

Confidence level: 7.56e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-Methylaniline

Measured: 191

Predicted: 109

[Image not found](#)

4-Vinylpyridine

Measured: 15.1

Predicted: 43.8

[Image not found](#)

3-Nitroaniline

Measured: 53.7

Predicted: 73.4

[Image not found](#)

Acetophenone

Measured: 63.1

Predicted: 67.9

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3-Methylaniline

Measured: 33.9

Predicted: 33.3