

Benzoic acid, 4-methoxy-
100-09-4 | DTXSID4059205

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: 50.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.16e-01

Confidence level: 8.31e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-Methyl-N'-phenylurea

Measured: 19.5

Predicted: 29.8

[Image not found](#)

Methyl phenylcarbamate

Measured: 53.7

Predicted: 59.1

[Image not found](#)

Methyl N-(3-chlorophenyl)carbamate

Measured: 141

Predicted: 94.1

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(2-Chlorophenyl)urea

Measured: 40.7

Predicted: 51.3