

Phenoxyacetic acid
122-59-8 | DTXSID9025873

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: 35.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.86e-01

Confidence level: 8.29e-01

Nearest Neighbors from the Training Set

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N-Methyl-N'-phenylurea

Measured: 19.5

Predicted: 29.8

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Urea, 1-(p-fluorophenyl)-

Measured: 33.1

Predicted: 49.6

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(2-Chlorophenyl)urea

Measured: 40.7

Predicted: 51.3

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Methyl phenylcarbamate

Measured: 53.7

Predicted: 59.1