

1-Phenylurea
64-10-8 | DTXSID8042507

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: 34.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.53e-01

Confidence level: 6.81e-01

Nearest Neighbors from the Training Set

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1-Phenylurea

Measured: 22.4

Predicted: 34.2

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4-Aminobenzoic acid

Measured: 316

Predicted: 96.6

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(2-Chlorophenyl)urea

Measured: 40.7

Predicted: 51.3

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Acetanilide

Measured: 26.9

Predicted: 40.2

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Urea, (3-methylphenyl)-

Measured: 36.3

Predicted: 37.2