

Phenacetin
62-44-2 | DTXSID1021116

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: 81.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.74e-01

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

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Propham

Measured: 67.6

Predicted: 83.2

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Propyl N-phenylcarbamate

Measured: 115

Predicted: 120

[Image not found](#)

N-Cyclopropyl-N'-phenylurea

Measured: 55.0

Predicted: 74.0

[Image not found](#)

Butyl benzoate

Measured: 126

Predicted: 76.3

[Image not found](#)

Carbamic acid, phenyl-, ethyl ester

Measured: 66.1

Predicted: 62.6