

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.49e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.60e-01

Confidence level: 4.41e-01

Nearest Neighbors from the Training Set

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Thiotepa

Measured: 1.00

Predicted: 2.48e-01

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Acetamide, 2-cyano-N-phenyl-

Measured: 1.87e-03

Predicted: 3.42e-01

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Fenuron

Measured: 2.45e-02

Predicted: 2.70e-01

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Phenazone

Measured: 2.73e-01

Predicted: 1.63