

Phenol
108-95-2 | DTXSID5021124

Model Performance

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: 1.48 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.92e-01

Confidence level: 7.08e-01

Nearest Neighbors from the Training Set

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2,3-Dibromopropanol

Measured: 2.39e-01

Predicted: 3.43e-01

[Image not found](#)

Dimercaprol

Measured: 7.00e-01

Predicted: 6.54e-01

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3-Bromo-1-propanol

Measured: 1.02

Predicted: 1.67

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2-Bromo-1-ethanol

Measured: 8.00

Predicted: 7.60

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2-Mercaptoethanol

Measured: 12.8

Predicted: 7.96