

Phenol
108-95-2 | DTXSID5021124

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.80

Global applicability domain: Inside

Local applicability domain index: 6.65e-01

Confidence level: 8.10e-01

Nearest Neighbors from the Training Set

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Phenol

Measured: 1.46

Predicted: 1.80

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o-Cresol

Measured: 1.95

Predicted: 2.10

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p-Cresol

Measured: 1.94

Predicted: 2.10

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m-Cresol

Measured: 1.96

Predicted: 2.12

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4-Fluorophenol

Measured: 1.77

Predicted: 2.08