

Phenol
108-95-2 | DTXSID5021124

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.98

Global applicability domain: Inside

Local applicability domain index: 6.10e-01

Confidence level: 6.95e-01

Nearest Neighbors from the Training Set

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Methyl tert-butyl ether

Measured: 1.51

Predicted: 3.67

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tert-Butyl alcohol

Measured: 5.01

Predicted: 4.48

Image not found

Diethyl ether

Measured: 5.37

Predicted: 4.72

Image not found

Triethylamine

Measured: 4.90

Predicted: 5.95

Image not found

Benzothiazole

Measured: 7.59

Predicted: 6.05