

Phenol
108-95-2 | DTXSID5021124

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 33.4 °C

Global applicability domain: Inside

Local applicability domain index: 7.97e-01

Confidence level: 5.60e-01

Nearest Neighbors from the Training Set

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Phenol

Measured: 40.9

Predicted: 33.4

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p-Cresol

Measured: 35.5

Predicted: 27.8

Image not found

m-Cresol

Measured: 11.8

Predicted: 18.9

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4-Ethenyl-phenol

Measured: 73.5

Predicted: 43.7

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Benzyl alcohol

Measured: -15.2

Predicted: 19.8