

Phenol
108-95-2 | DTXSID5021124

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.20e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.63e-01

Confidence level: 7.72e-01

Nearest Neighbors from the Training Set

Image not found

Cyclohexanone

Measured: 3.50e-01

Predicted: 5.20

Image not found

m-Xylene

Measured: 1.10e-01

Predicted: 8.96

Image not found

4-Chlorotoluene

Measured: 1.10e-01

Predicted: 3.64

Image not found

3-Chloroaniline

Measured: 1.25e-01

Predicted: 9.03e-02

Image not found

4-Chloroaniline

Measured: 8.90e-02

Predicted: 6.91e-02