

Phenol, 4-chloro-2-methoxy-
16766-30-6 | DTXSID0074974

Model Performance

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: 8.05e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.85e-01

Confidence level: 6.12e-01

Nearest Neighbors from the Training Set

Image not found

cis-1,2-Dimethylcyclopentane

Measured: 4.44e-03

Predicted: N/A

Image not found

Dichloromethylphenylsilane

Measured: 1.96e-02

Predicted: 7.56e-01

Image not found

2-Nitrophenol

Measured: 1.03e-01

Predicted: 2.18e-02

Image not found

Ethanol, 2-(phenylamino)-

Measured: 7.00e-03

Predicted: 2.79e-03

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Isolane

Measured: 1.99e-04

Predicted: 1.58e-03