

2-Methyl-p-benzoquinone
553-97-9 | DTXSID8060290

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.09e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.10e-01

Confidence level: 5.20e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Octadecanethiol

Measured: 1.02

Predicted: 1.14e-06

[Image not found](#)

Phenylhydrazine

Measured: 2.80e-02

Predicted: 8.40e-03

[Image not found](#)

4-Chlorophenol

Measured: 9.00e-02

Predicted: 9.27e-02

[Image not found](#)

4-Methylbenzyl chloride

Measured: 3.13e-01

Predicted: 5.21e-01

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N,N,4-Trimethylaniline

Measured: 1.57e-02

Predicted: 2.64e-01