

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.89

Global applicability domain: Inside

Local applicability domain index: 5.53e-01

Confidence level: 6.66e-01

Nearest Neighbors from the Training Set

Image not found

4-Methylimidazolidine-2-thione

Measured: 10.0

Predicted: 4.59

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1,4-Dioxane

Measured: 5.01e-01

Predicted: 1.06

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Diethyl ether

Measured: 5.37

Predicted: 4.72

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Morpholine

Measured: 2.82

Predicted: 1.87

Image not found

Ethylene thiourea

Measured: 1.82

Predicted: 1.85