

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 30.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.60e-01

Confidence level: 8.40e-01

Nearest Neighbors from the Training Set

Image not found

Benzamide

Measured: 28.8

Predicted: 29.7

Image not found

3-Pyridinecarbonitrile

Measured: 36.3

Predicted: 25.0

Image not found

2-(Pyridin-2-yl)ethanol

Measured: 28.2

Predicted: 35.9

Image not found

4-Hydroxybenzoic acid

Measured: 26.9

Predicted: 76.6

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Benzoic acid

Measured: 31.6

Predicted: 35.5