

1,4-Naphthoquinone
130-15-4 | DTXSID5040704

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.43

Global applicability domain: Inside

Local applicability domain index: 6.46e-01

Confidence level: 6.24e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,3-Indandione

Measured: 0.61

Predicted: 1.65

[Image not found](#)

1,4-Naphthoquinone

Measured: 1.71

Predicted: 1.43

[Image not found](#)

2-Hydroxy-1,4-naphthoquinone

Measured: 1.38

Predicted: 1.34

[Image not found](#)

Menadione

Measured: 2.20

Predicted: 1.65

[Image not found](#)

Benzaldehyde, 3-bromo-4-hydroxy-

Measured: 1.83

Predicted: 1.31