

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 115 °C

Global applicability domain: Inside

Local applicability domain index: 7.78e-01

Confidence level: 6.10e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,4-Naphthoquinone

Measured: 129

Predicted: 115

[Image not found](#)

Menadione

Measured: 107

Predicted: 108

[Image not found](#)

2,3-Dimethyl-1,4-naphthoquinone

Measured: 127

Predicted: 108

[Image not found](#)

1,2-Diphenylethanedione

Measured: 94.8

Predicted: 100

[Image not found](#)

1,3-Diphenyl-1,3-propanedione

Measured: 70.5

Predicted: 93.8