

1,2-Naphthalenedione, 3,8-dimethyl-5-(1-methylethyl)-
5574-34-5 | DTXSID80204286

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.89 | 0.25 | 0.88 | 0.26 | 0.75 | 0.38 |

Model Results

Predicted value: 4.65 days

Global applicability domain: Outside

Local applicability domain index: 3.91e-01

Confidence level: 8.76e-01

Nearest Neighbors from the Training Set

Image not found

1-Methyl-2-propylbenzene

Measured: 12.5

Predicted: 3.17

Image not found

9-Ethyl-9H-fluorene

Measured: 2330

Predicted: N/A

Image not found

5-Methylindan

Measured: 4.93

Predicted: 2.25

Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: 24.3

Predicted: 3.89

Image not found

3-Ethyltoluene

Measured: 12.5

Predicted: 3.26