

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

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: 10.2

Global applicability domain: Inside

Local applicability domain index: 4.82e-01

Confidence level: 6.00e-01

Nearest Neighbors from the Training Set

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Disulfoton

Measured: 219

Predicted: 151

[Image not found](#)

O,O-Diethyl dithiophosphate

Measured: 5.01

Predicted: 5.43

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Thiram

Measured: 3.39

Predicted: 3.91

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Isophorone

Measured: 2.00

Predicted: 3.19

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Menthol

Measured: 10.8

Predicted: 23.5

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(1R,2S,5R)-(-)-Menthol

Measured: 10.8

Predicted: 23.5