

propan-2-yl naphthalen-1-ylacetate
68360-82-7 | DTXSID60286262

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.07

Global applicability domain: Inside

Local applicability domain index: 9.33e-01

Confidence level: 8.22e-01

Nearest Neighbors from the Training Set

Image not found

1,2,3,4-Tetrachloronaphthalene

Measured: 8.30

Predicted: 8.41

Image not found

2,3-Dichlorodibenzo-4-dioxin

Measured: 8.50

Predicted: 8.49

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4,4'-Dichlorobiphenyl

Measured: 7.68

Predicted: 7.38

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2,2'-Dichlorobiphenyl

Measured: 7.18

Predicted: 7.38