

Indene
95-13-6 | DTXSID8042052

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.21e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.63e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

Image not found

5-Ethylidene-2-norbornene

Measured: 7.40e-05

Predicted: 2.32e-04

Image not found

1,4-Dithiane

Measured: 2.50e-02

Predicted: 1.47e-02

Image not found

Diethyl disulphide

Measured: 2.45e-03

Predicted: 3.63e-03

Image not found

Ethane, 1,2-diiodo-

Measured: 6.06e-04

Predicted: 1.27e-03