

Propylbenzene
103-65-1 | DTXSID3042219

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: 2.20e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.39e-01

Confidence level: 6.20e-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

4-Vinylcyclohexene

Measured: 4.62e-04

Predicted: 3.42e-04

Image not found

Bromocyclohexane

Measured: 5.08e-03

Predicted: 2.15e-03

Image not found

1-Heptanethiol

Measured: 7.00e-05

Predicted: 6.62e-05

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Terpinolene

Measured: 6.97e-05

Predicted: 6.64e-05