

1-Methyl-2-propylbenzene
1074-17-5 | DTXSID4061466

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: 5.11e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.65e-01

Confidence level: 8.37e-01

Nearest Neighbors from the Training Set

Image not found

Heptane, 1-iodo-

Measured: 1.55e-05

Predicted: 2.40e-05

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

Image not found

gamma-Terpinene

Measured: 6.37e-05

Predicted: 4.78e-05

Image not found

Limonene

Measured: 7.77e-05

Predicted: 5.10e-05

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D-Limonene

Measured: 7.77e-05

Predicted: 5.10e-05