

Pentane
109-66-0 | DTXSID2025846

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: 6.69e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.05e-01

Confidence level: 8.57e-01

Nearest Neighbors from the Training Set

Image not found

Pentane

Measured: 5.27e-04

Predicted: 6.69e-04

Image not found

2-Methylbutane

Measured: 6.76e-04

Predicted: 8.06e-04

Image not found

Hexene

Measured: 5.94e-04

Predicted: 6.01e-04

Image not found

1-Hexene

Measured: 5.94e-04

Predicted: 6.46e-04

Image not found

1-Pentene

Measured: 2.11e-03

Predicted: 2.15e-03