

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 34.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.42e-01

Confidence level: 7.73e-01

Nearest Neighbors from the Training Set

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Toluene

Measured: 117

Predicted: 87.4

[Image not found](#)

Benzene

Measured: 56.2

Predicted: 50.5

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Phenol

Measured: 26.9

Predicted: 57.3

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1-Pentanol

Measured: 5.01

Predicted: 7.31

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Aniline

Measured: 39.8

Predicted: 53.3