

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 300 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.89e-01

Confidence level: 8.61e-01

Nearest Neighbors from the Training Set

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2-Methylpyrazine

Measured: 514

Predicted: 1.86

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Ethane, 1,2-dibromo-1,1-dichloro-

Measured: 319

Predicted: 1.55

[Image not found](#)

1,1,2,2-Tetrabromoethane

Measured: 235

Predicted: 7.26e-02

[Image not found](#)

1-Bromopentane

Measured: 151

Predicted: 7.15