

1,1-dimethoxyhexan-2-one
6344-10-1 | DTXSID70287285

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: 8.19e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.68e-01

Confidence level: 7.97e-01

Nearest Neighbors from the Training Set

Image not found

Nonanoic acid

Measured: 3.75e-01

Predicted: 1.91e-03

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Heptanoic acid

Measured: 2.34

Predicted: 6.20e-03

Image not found

Acetic acid, chloro-, 1-methylethyl ester

Measured: 2.69e-01

Predicted: 6.23

Image not found

bis(2-Chloro-1-methylethyl) ether

Measured: 3.92

Predicted: 1.62

Image not found

4-Bromophenol

Measured: 4.10e-01

Predicted: 2.33e-02