

Ethyl hydrogen glutarate
1070-62-8 | DTXSID20147865

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: 1.74e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.54e-01

Confidence level: 3.10e-01

Nearest Neighbors from the Training Set

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1-Naphthylamine

Measured: 4.00e-01

Predicted: 9.37e-04

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2-Butanone, 1-bromo-

Measured: 1.26e-01

Predicted: 7.89

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Phenyl phosphorodichloridate

Measured: 5.23e-02

Predicted: 1.16e-02

[Image not found](#)

3-Ethyl-2,2-dimethylpentane

Measured: 5.40e-06

Predicted: 11.5

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Piperophos

Measured: 5.48e-02

Predicted: 3.95e-07