

Diethyl butanedioate
123-25-1 | DTXSID2038732

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: 7.43e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.25e-01

Confidence level: 7.32e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Phenyl acetate

Measured: 4.39e-02

Predicted: 3.39e-01

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Fumaryl chloride

Measured: 6.04e-02

Predicted: 1.29

[Image not found](#)

N-Methoxymethylamine

Measured: 1.80e-01

Predicted: 122

[Image not found](#)

8-Pentadecanone

Measured: 1.61e-01

Predicted: 1.58e-03

[Image not found](#)

Ethyl acrylate

Measured: 1.05e-01

Predicted: 32.1