

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.48e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.10e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

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Diethyl butanedioate

Measured: 1.10e-01

Predicted: 1.48e-01

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Dimethyl adipate

Measured: 3.44e-02

Predicted: 1.69e-01

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Propylene glycol diacetate

Measured: 6.24e-01

Predicted: 3.94e-01

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1,3-Propanediol, diacetate

Measured: 6.24e-01

Predicted: 4.12e-01

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ethyl 2-acetyloxypropanoate

Measured: 2.00e-01

Predicted: 2.26e-01