

Dimethyl adipate
627-93-0 | DTXSID8025096

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: 1.69e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.09e-01

Confidence level: 5.20e-01

Nearest Neighbors from the Training Set

Image not found

Dimethyl adipate

Measured: 3.44e-02

Predicted: 1.69e-01

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Diethyl butanedioate

Measured: 1.10e-01

Predicted: 1.48e-01

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1,3-Propanediol, diacetate

Measured: 6.24e-01

Predicted: 4.12e-01

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2-(2-Ethoxyethoxy)ethyl acetate

Measured: 5.68

Predicted: 7.71e-01

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Propylene glycol diacetate

Measured: 6.24e-01

Predicted: 3.94e-01