

Dimethyl glutarate
1119-40-0 | DTXSID3025122

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: 4.48e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.32e-01

Confidence level: 7.03e-01

Nearest Neighbors from the Training Set

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Dimethyl glutarate

Measured: 3.68e-01

Predicted: 4.48e-01

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1,3-Propanediol, diacetate

Measured: 6.24e-01

Predicted: 4.12e-01

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Propylene glycol diacetate

Measured: 6.24e-01

Predicted: 3.94e-01

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1,2-Ethanediol diacetate

Measured: 1.22

Predicted: 4.77e-01

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Propanoic acid, 2-(1-oxopropoxy)-, methyl ester

Measured: 1.37e-01

Predicted: 2.58e-01