

Dimethyl decanedioate
106-79-6 | DTXSID1026740

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: 9.85e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.09e-01

Confidence level: 7.43e-01

Nearest Neighbors from the Training Set

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Dimethyl decanedioate

Measured: 5.21e-04

Predicted: 9.85e-04

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Diethyl suberate

Measured: 2.95e-03

Predicted: 1.82e-03

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Dibutyl butanedioate

Measured: 9.99e-04

Predicted: 1.53e-03

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Nonanedioic acid, diethyl ester

Measured: 1.02e-03

Predicted: 9.14e-04

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Dibutyl maleate

Measured: 2.19e-03

Predicted: 1.60e-03