

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 1.98 °C

Global applicability domain: Inside

Local applicability domain index: 9.34e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

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Dimethyl decanedioate

Measured: 38.0

Predicted: 1.98

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Diethyl suberate

Measured: 5.90

Predicted: -3.58

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Dipropyl hexanedioate

Measured: -15.7

Predicted: -6.62

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Dibutyl butanedioate

Measured: -29.2

Predicted: -25.5

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Nonanedioic acid, diethyl ester

Measured: -18.5

Predicted: -11.8