

Dimethyl succinate
106-65-0 | DTXSID5025152

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.94e-01

Global applicability domain: Inside

Local applicability domain index: 6.81e-01

Confidence level: 8.57e-01

Nearest Neighbors from the Training Set

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Dimethyl succinate

Measured: 0.35

Predicted: 3.94e-01

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Dimethyl glutarate

Measured: 0.62

Predicted: 7.46e-01

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Diethyl propanedioate

Measured: 0.96

Predicted: 8.73e-01

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Dimethyl malonate

Measured: -0.0500

Predicted: -0.0121

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Dimethyl maleate

Measured: 0.22

Predicted: 1.92e-01

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2-Butenedioic acid (2E)-, 1,4-dimethyl ester

Measured: 0.22

Predicted: 1.92e-01