

Butanedioic acid, ethyl methyl ester
627-73-6 | DTXSID7074327

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: 8.52e-01

Global applicability domain: Inside

Local applicability domain index: 7.05e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

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Diethyl propanedioate

Measured: 0.96

Predicted: 8.73e-01

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Dimethyl glutarate

Measured: 0.62

Predicted: 7.46e-01

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Diethyl butanedioate

Measured: 1.20

Predicted: 1.04

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Dimethyl succinate

Measured: 0.35

Predicted: 3.94e-01

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Dimethyl adipate

Measured: 1.03

Predicted: 1.03