

Propanedioic acid, diethyl-
510-20-3 | DTXSID9060150

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: 1.87 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.19e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

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n-Pentylmalonic acid

Measured: 3.91

Predicted: 6.99e-01

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n-Propylmalonic acid

Measured: 4.79

Predicted: 5.06

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Hexylmalonic acid

Measured: 2.20e-02

Predicted: 2.58e-02

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Ethylmalonic acid

Measured: 5.39

Predicted: 5.64