

Heptanedioic acid
111-16-0 | DTXSID5021598

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: 6.46e-01

Global applicability domain: Inside

Local applicability domain index: 6.85e-01

Confidence level: 8.16e-01

Nearest Neighbors from the Training Set

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Heptanedioic acid

Measured: 0.61

Predicted: 6.46e-01

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Hexanedioic acid

Measured: 0.08

Predicted: 6.25e-02

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2,2-Dimethylpentanedioic acid

Measured: 0.67

Predicted: 7.43e-01

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4-oxo-2-propylpentanoic acid

Measured: 1.31

Predicted: 1.27

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Isovaleric acid

Measured: 1.16

Predicted: 1.30