

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.47e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.36e-01

Confidence level: 5.26e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Heptanedioic acid

Measured: 3.12e-01

Predicted: 1.47e-01

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Octanedioic acid

Measured: 6.79e-02

Predicted: 4.83e-02

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Propionic acid, 3,3'-diselenodi-

Measured: 5.39e-03

Predicted: 1.65e-02