

4H-Pyran-4-one, tetrahydro-3,5-bis(hydroxymethyl)-
67845-26-5 | DTXSID3028342

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: 7.30e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.60e-01

Confidence level: 5.83e-01

Nearest Neighbors from the Training Set

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Butyl 3-hydroxypropanoate

Measured: 5.13e-02

Predicted: 1.05e-01

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3-Methyl-2-oxoxolane-3-carboxylic acid

Measured: 6.94

Predicted: 5.23

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Propanal, 3-hydroxy-2,2-dimethyl-

Measured: 4.70e-01

Predicted: 1.07

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L-Threonine

Measured: 9.76e-01

Predicted: 1.26

Image not found

L-Threonine

Measured: 9.76e-01

Predicted: 1.26