

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 134 °C

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 4.96e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Kojic acid

Measured: 154

Predicted: 147

[Image not found](#)

Hydroperoxide, (1,4-phenylenebis(1-methylethylidene))bis-

Measured: 141

Predicted: 136

[Image not found](#)

Guaifenesin

Measured: 78.5

Predicted: 80.2

[Image not found](#)

2-Hydroxy-1-[4-(2-hydroxyethoxy)phenyl]-2-methylpropan-1-one

Measured: 89.0

Predicted: 100