

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 276 °C

Global applicability domain: Inside

Local applicability domain index: 4.44e-01

Confidence level: 6.95e-01

Nearest Neighbors from the Training Set

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Tetraethylene glycol

Measured: 328

Predicted: 318

Image not found

4-Methylcatechol

Measured: 251

Predicted: 257

Image not found

1,2-Benzenediol, 3-methyl-

Measured: 241

Predicted: 257

Image not found

Styrene glycol

Measured: 273

Predicted: 267

Image not found

Diethyl L-tartrate

Measured: 280

Predicted: 284