

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 9.42×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.55×10^{-1}

Confidence level: 7.69×10^{-1}

Nearest Neighbors from the Training Set

[Image not found](#)

Diacetone alcohol

Measured: 4.00×10^{-12}

Predicted: 6.56×10^{-12}

[Image not found](#)

2-Butanone, 1-hydroxy-

Measured: 7.70×10^{-12}

Predicted: 7.95×10^{-12}

[Image not found](#)

Acetoin

Measured: 1.03×10^{-11}

Predicted: 8.75×10^{-12}