

2,2-Bis(bromomethyl)-1,3-propanediol
3296-90-0 | DTXSID9020164

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.49 days

Global applicability domain: Outside

Local applicability domain index: 3.48e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

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Ethylbenzene

Measured: 120

Predicted: 6.21

[Image not found](#)

Propylbenzene

Measured: 24.3

Predicted: 4.02

[Image not found](#)

5-Methylindan

Measured: 4.93

Predicted: 2.25

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1,3-Diethylbenzene

Measured: 88.3

Predicted: 5.36

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4-Ethyltoluene

Measured: 24.3

Predicted: 3.95