

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

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 149 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.69e-01

Confidence level: 7.31e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Clopyralid

Measured: 36.3

Predicted: 37.7

[Image not found](#)

3-Bromophenylurea

Measured: 132

Predicted: 114

[Image not found](#)

4-Bromo-m-toluidine

Measured: 182

Predicted: 173

[Image not found](#)

Acetamide, N-(3-bromophenyl)-
(9CI)

Measured: 102

Predicted: 77.2

[Image not found](#)

Zineb

Measured: 1000

Predicted: 398