

4,4'-(Propane-2,2-diyl)di(¹³C₆)phenol
263261-65-0 | DTXSID10675703

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	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.48

Global applicability domain: Inside

Local applicability domain index: 5.44e-01

Confidence level: 7.92e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Cyclohexylphenylacetic acid

Measured: 3.91

Predicted: 3.90

[Image not found](#)

Bisphenol A

Measured: 3.32

Predicted: 3.20

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4-Hexylresorcinol

Measured: 3.45

Predicted: 3.66