

2,2'-Dihydroxybenzophenone
835-11-0 | DTXSID8022404

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.23e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.34e-01

Confidence level: 5.31e-01

Nearest Neighbors from the Training Set

[Image not found](#)

3,5-Dibromo-2-hydroxycyclohepta-2,4,6-trien-1-one

Measured: 3.14e-04

Predicted: 6.20e-04

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2,4,6-Cycloheptatrien-1-one, 3-bromo-2-hydroxy-

Measured: 3.67e-03

Predicted: 2.27e-03

[Image not found](#)

5-Bromo-2-hydroxycyclohepta-2,4,6-trien-1-one

Measured: 2.74e-04

Predicted: 9.82e-04

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4-(1-Naphthyl)-4-oxobutanoic acid

Measured: 3.29e-04

Predicted: 3.91e-03