

4,4'-[(1,3-<sup>13</sup>C<sub>2</sub>)Propane-2,2-diyl]diphenol  
263261-64-9 | DTXSID30747173

## 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:** 3.68e-03 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 3.64e-01

**Confidence level:** 4.63e-01

## Nearest Neighbors from the Training Set

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1,3-Naphthalenediol

**Measured:** 1.12e-02

**Predicted:** 2.01e-02

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1,5-Dihydroxynaphthalene

**Measured:** 1.03e-03

**Predicted:** 8.87e-03

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3-Amino-3-(naphthalen-1-yl)propanoic acid

**Measured:** 2.57e-02

**Predicted:** 1.36e-02

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2,3-Dihydroxynaphthalene

**Measured:** 1.83e-03

**Predicted:** 3.03e-02