

4,4'-[(1,3-¹³C₂)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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 24.1

Global applicability domain: Inside

Local applicability domain index: 4.92e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

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Oxydisulfoton

Measured: 1.00

Predicted: 1.63

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Disulfoton

Measured: 219

Predicted: 151

[Image not found](#)

Parathion

Measured: 97.7

Predicted: 22.3

[Image not found](#)

O,O-Diethyl dithiophosphate

Measured: 5.01

Predicted: 5.43

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Methyl parathion

Measured: 85.1

Predicted: 14.5