

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 144 °C

Global applicability domain: Inside

Local applicability domain index: 9.10e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

Image not found

Bisphenol A

Measured: 153

Predicted: 144

Image not found

4,4'-Propane-1,1-diylidiphenol

Measured: 132

Predicted: 133

Image not found

phenol, 4,4'-butylidenebis-

Measured: 137

Predicted: 142

Image not found

Bisphenol B

Measured: 121

Predicted: 140

Image not found

meso-Hexestrol

Measured: 187

Predicted: 157