

2,2'-Methylenebis(1,3-dioxolane)
4405-17-8 | DTXSID90196027

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: -8.85 °C

Global applicability domain: Inside

Local applicability domain index: 4.85e-01

Confidence level: 6.28e-01

Nearest Neighbors from the Training Set

Image not found

1,4,7,10-Tetraoxacyclododecane

Measured: 16.0

Predicted: 9.14

Image not found

Pinacolyl
methylphosphonofluoridate

Measured: -42.0

Predicted: -48.2

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Ethyl 2,4-dioxovalerate

Measured: 18.0

Predicted: 27.4

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2-Propene-1,1-diol diacetate

Measured: -37.6

Predicted: -3.57

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Diethyl 2-butynedioate

Measured: 1.50

Predicted: 6.71