

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.46e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.15e-01

Confidence level: 5.36e-01

Nearest Neighbors from the Training Set

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1-Bromodecane

Measured: 4.03e-02

Predicted: 2.76e-02

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2-Undecanone

Measured: 9.89e-02

Predicted: 6.59e-02

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Octanal

Measured: 4.00e-02

Predicted: 9.32e-01

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Phosmet

Measured: 2.30e-02

Predicted: 5.53e-07

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4-Thiocresol

Measured: 1.48e-03

Predicted: 7.46e-01