

2,2-Dimethyl-1,3-dioxolane
2916-31-6 | DTXSID10183419

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: 47.0 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.58e-01

Confidence level: 8.58e-01

Nearest Neighbors from the Training Set

Image not found

Butyl acetate

Measured: 38.1

Predicted: 16.4

Image not found

2-Ethyl-2-hexenal

Measured: 79.0

Predicted: 1.35

Image not found

Fluorobenzene

Measured: 34.1

Predicted: 58.3

Image not found

Ethyl butyrate

Measured: 27.6

Predicted: 14.7

Image not found

3-Methyl-3-pentanol

Measured: 102

Predicted: 4.48