

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 18.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 6.82e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Dioxane

Measured: 17.0

Predicted: 13.2

Image not found

3-Methylaniline

Measured: 33.9

Predicted: 33.3

Image not found

Pyridine

Measured: 39.8

Predicted: 20.1

Image not found

3-Pyridinecarbonitrile

Measured: 36.3

Predicted: 25.0

Image not found

2,2'-Bioxirane

Measured: 2.51

Predicted: 4.97