

2-(1-Hydroxy-1-methylethyl-2-methyl-1,3-dioxane
39239-96-8 | DTXSID80192497

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: 1.10e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.24e-01

Confidence level: 3.63e-01

Nearest Neighbors from the Training Set

Image not found

Decanal

Measured: 2.19e-02

Predicted: 1.51e-01

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Tetraethylenepentamine

Measured: 1.18e-03

Predicted: 1.09e-06

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1-Octanethiol

Measured: 1.26e-01

Predicted: 3.49e-01

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Heptanal

Measured: 2.50e-01

Predicted: 2.33

Image not found

Quinuclidine

Measured: 107

Predicted: 2.06