

1,4-Dioxane
123-91-1 | DTXSID4020533

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.157

Global applicability domain: Inside

Local applicability domain index: 5.64e-01

Confidence level: 6.86e-01

Nearest Neighbors from the Training Set

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1,4-Dioxane

Measured: -0.270

Predicted: -0.157

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Morpholine

Measured: -0.860

Predicted: -0.646

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Ethanamine, N-methyl-

Measured: 0.15

Predicted: 1.26e-01

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Diethyl ether

Measured: 0.89

Predicted: 9.83e-01