

2,4,8,10-Tetraoxaspiro[5.5]undecane
126-54-5 | DTXSID2059566

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.44e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.63e-01

Confidence level: 5.17e-01

Nearest Neighbors from the Training Set

Image not found

2,5-dimethoxy-2,5-dimethyl-1,4-dioxane

Measured: 5.68e-02

Predicted: 2.72e-01

Image not found

Bis(2-methoxyethyl) ether

Measured: 7.45

Predicted: 4.34

Image not found

Dimethyl glutarate

Measured: 3.68e-01

Predicted: 4.48e-01

Image not found

2-(2-Ethoxyethoxy)ethyl acetate

Measured: 5.68

Predicted: 7.71e-01