

1,5,7,11-Tetraoxaspiro[5.5]undecane
24472-02-4 | DTXSID1066994

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: 9.41e-01

Global applicability domain: Inside

Local applicability domain index: 5.50e-01

Confidence level: 8.24e-01

Nearest Neighbors from the Training Set

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Diethyl butanedioate

Measured: 1.20

Predicted: 1.04

[Image not found](#)

Diethyl propanedioate

Measured: 0.96

Predicted: 8.73e-01

[Image not found](#)

Dimethyl adipate

Measured: 1.03

Predicted: 1.03

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2-Propene-1,1-diol diacetate

Measured: 0.78

Predicted: 7.05e-01

[Image not found](#)

Dimethyl glutarate

Measured: 0.62

Predicted: 7.46e-01