

3-Deoxy-manno-oct-2-ulopyranosonic acid
10149-14-1 | DTXSID80143949

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: 8.11e-11 mmHg

Global applicability domain: Outside

Local applicability domain index: 2.15e-01

Confidence level: 2.73e-01

Nearest Neighbors from the Training Set

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Lepidine

Measured: 8.02e-14

Predicted: 9.90e-03

Image not found

4-Chloro-3-methylphenol

Measured: 1.50e-12

Predicted: 5.35e-02

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Perflutren

Measured: 1.66e-08

Predicted: 7890

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2,2,5,5-Tetramethylhexane

Measured: 9.80e-08

Predicted: 7.94

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Benz(a)anthracene

Measured: 1.97e-10

Predicted: 2.14e-08