

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

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 1.14 | 0.85 | 1.12 | 0.83 | 1.23 |

Model Results

Predicted value: 1.07e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.24e-01

Confidence level: 8.13e-01

Nearest Neighbors from the Training Set

Image not found

Bornyl acetate

Measured: 1.39e-11

Predicted: 1.36e-11

Image not found

2-Ethoxyethyl isobutyrate

Measured: 1.35e-11

Predicted: 1.28e-11

Image not found

Ethyl lactate

Measured: 3.90e-12

Predicted: 4.80e-12

Image not found

Dimethyl adipate

Measured: 8.40e-12

Predicted: 6.84e-12

Image not found

Ethyl 3-ethoxypropionate

Measured: 2.29e-11

Predicted: 1.63e-11