

Methyl alpha-D-glucopyranoside
97-30-3 | DTXSID7026605

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.89 | 0.25 | 0.88 | 0.26 | 0.75 | 0.38 |

Model Results

Predicted value: 3.54 days

Global applicability domain: Outside

Local applicability domain index: 3.86e-01

Confidence level: 9.36e-01

Nearest Neighbors from the Training Set

Image not found

1-Methyl-2-propylbenzene

Measured: 12.5

Predicted: 3.17

Image not found

Propylbenzene

Measured: 24.3

Predicted: 4.02

Image not found

3-Ethyltoluene

Measured: 12.5

Predicted: 3.26

Image not found

1-Ethyl-2-methylbenzene

Measured: 24.3

Predicted: 3.88

Image not found

4-Ethyltoluene

Measured: 24.3

Predicted: 3.95