

Butyl ether
142-96-1 | DTXSID1022007

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: 3.81 days

Global applicability domain: Outside

Local applicability domain index: 3.98e-01

Confidence level: 8.08e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2-Methylheptane

Measured: 12.5

Predicted: 3.99

[Image not found](#)

2-Methylhexane

Measured: 12.5

Predicted: 5.54

[Image not found](#)

2,4-Dimethylheptane

Measured: 61.9

Predicted: 4.29

[Image not found](#)

4-Methyloctane

Measured: 40.7

Predicted: 3.58