

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 |
| 0.84 | 0.55 | 0.85 | 0.53 | 0.83 | 0.64 |

Model Results

Predicted value: 32.3

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 5.81e-01

Nearest Neighbors from the Training Set

[Image not found](#)

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Measured: 72.4

Predicted: 32.3

[Image not found](#)

cis-Nanophine

Measured: 5.01

Predicted: 6.12

[Image not found](#)

Quinoline

Measured: 3.80

Predicted: 6.66

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N-Ethylaniline

Measured: 12.9

Predicted: 5.70