

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 |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 2.99

Global applicability domain: Inside

Local applicability domain index: 6.01e-01

Confidence level: 6.78e-01

Nearest Neighbors from the Training Set

Image not found

Butyl ether

Measured: 3.21

Predicted: 2.99

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Propane, 1,1'-oxybis[2-methyl-

Measured: 2.78

Predicted: 2.92

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Ethylene glycol dibutyl ether

Measured: 2.48

Predicted: 2.62

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N-Butyl-1-butanamine

Measured: 2.83

Predicted: 2.60

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1-Ethoxybutane

Measured: 2.03

Predicted: 1.86