

Butyl nitrate
928-45-0 | DTXSID70239143

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: 1.60

Global applicability domain: Inside

Local applicability domain index: 5.89e-01

Confidence level: 3.70e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Butyl nitrate

Measured: 2.15

Predicted: 1.60

[Image not found](#)

Isoamyl nitrate

Measured: 2.84

Predicted: 1.84

[Image not found](#)

Isopropylamine

Measured: 0.26

Predicted: 3.49e-01

[Image not found](#)

2-Butanone oxime

Measured: 0.63

Predicted: 1.48