

tert-Butyl nitrite
540-80-7 | DTXSID10202316

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.87 | 0.81 | 0.87 | 0.82 | 0.86 | 0.86 |

Model Results

Predicted value: 7.28e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.46e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

Image not found

Methyl tert-butyl ether

Measured: 5.78e-01

Predicted: 3.76e-01

Image not found

2-Methyl-2-ethoxypropane

Measured: 1.17e-01

Predicted: 5.28e-02

Image not found

Propane, 2-ethoxy-

Measured: 2.78e-01

Predicted: 2.38e-01

Image not found

1-Propene, 3,3'-oxybis-

Measured: 9.54e-01

Predicted: 6.49e-01

Image not found

2-Methoxyprop-1-ene

Measured: 13.9

Predicted: 2.31