

tert-Butyl nitrite
540-80-7 | DTXSID10202316

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.68 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.97e-01

Confidence level: 7.01e-01

Nearest Neighbors from the Training Set

Image not found

3-Mercaptopropanoic acid

Measured: 5.10

Predicted: 5.30e-02

Image not found

Diethoxymethane

Measured: 3.97

Predicted: 50.4

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N-Methylcarbamic acid, ethyl ester

Measured: 8.92e-01

Predicted: 1.51

Image not found

4-Methyl-1-pentene

Measured: 313

Predicted: 268

Image not found

2,4-Pentanedione

Measured: 1.36

Predicted: 3.07