

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.53

Global applicability domain: Inside

Local applicability domain index: 6.23e-01

Confidence level: 5.97e-01

Nearest Neighbors from the Training Set

[Image not found](#)

6-Aminocaproic acid

Measured: -2.95

Predicted: -2.71

[Image not found](#)

omega-Aminoenantic acid

Measured: -3.03

Predicted: -2.72

[Image not found](#)

2-Butanone oxime

Measured: 0.63

Predicted: 1.48

[Image not found](#)

5-Aminovaleric acid

Measured: -2.63

Predicted: -2.62