

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 74.7 °C

Global applicability domain: Inside

Local applicability domain index: 8.76e-01

Confidence level: 7.15e-01

Nearest Neighbors from the Training Set

[Image not found](#)

tert-Butyl nitrite

Measured: 63.0

Predicted: 74.7

[Image not found](#)

Isobutyl nitrite

Measured: 67.0

Predicted: 74.6

[Image not found](#)

N-Butylnitrite

Measured: 78.0

Predicted: 74.8