

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 24.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.23e-01

Confidence level: 6.19e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Phenol

Measured: 26.9

Predicted: 57.3

[Image not found](#)

Toluene

Measured: 117

Predicted: 87.4

[Image not found](#)

Benzene

Measured: 56.2

Predicted: 50.5

[Image not found](#)

Resorcinol

Measured: 9.55

Predicted: 28.3

[Image not found](#)

1-Butanol

Measured: 3.16

Predicted: 8.95