

Benzonitrile
100-47-0 | DTXSID7021491

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 6.30

Global applicability domain: Inside

Local applicability domain index: 6.02e-01

Confidence level: 5.81e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Diethyl ether

Measured: 5.37

Predicted: 4.72

[Image not found](#)

Methyl tert-butyl ether

Measured: 1.51

Predicted: 3.67

[Image not found](#)

Triethylamine

Measured: 4.90

Predicted: 5.95

[Image not found](#)

N,N-Dimethyl-1,2-dithiolan-4-amine

Measured: 52.5

Predicted: 17.5

[Image not found](#)

Benzothiazole

Measured: 7.59

Predicted: 6.05