

Benzonitrile  
100-47-0 | DTXSID7021491

### 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
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** -8.37 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 8.64e-01

**Confidence level:** 6.40e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Benzonitrile

**Measured:** -12.7

**Predicted:** -8.37

[Image not found](#)

2-Tolunitrile

**Measured:** -13.5

**Predicted:** -2.49

[Image not found](#)

3-Methylbenzonitrile

**Measured:** -23.0

**Predicted:** -2.44

[Image not found](#)

4-Methylbenzonitrile

**Measured:** 29.5

**Predicted:** -2.41

[Image not found](#)

Benzyl cyanide

**Measured:** -23.8

**Predicted:** -4.67