

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 199 °C

Global applicability domain: Inside

Local applicability domain index: 7.22e-01

Confidence level: 8.68e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Benzonitrile

Measured: 191

Predicted: 199

[Image not found](#)

2-Tolunitrile

Measured: 205

Predicted: 209

[Image not found](#)

3-Methylbenzonitrile

Measured: 213

Predicted: 210

[Image not found](#)

4-Methylbenzonitrile

Measured: 217

Predicted: 213