

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.59

Global applicability domain: Inside

Local applicability domain index: 5.98e-01

Confidence level: 7.63e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Benzonitrile

Measured: 1.56

Predicted: 1.59

[Image not found](#)

Benzonitrile, 3-fluoro-

Measured: 1.47

Predicted: 1.61

[Image not found](#)

m-Formylbenzonitrile

Measured: 1.18

Predicted: 1.23

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2-Tolunitrile

Measured: 2.21

Predicted: 1.73

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2-Hydroxybenzonitrile

Measured: 1.61

Predicted: 1.60