

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.44e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.43e-01

Confidence level: 8.25e-01

Nearest Neighbors from the Training Set

Image not found

4-Dimethylaminobenzaldehyde

Measured: 7.68e-01

Predicted: 4.24e-03

Image not found

Benzyl alcohol

Measured: 1.27

Predicted: 2.44e-01

Image not found

1,2-Diphenylhydrazine

Measured: 3.92e-01

Predicted: 2.66e-05

Image not found

alpha-Methylstyrene

Measured: 3.97e-01

Predicted: 2.24

Image not found

2,3-Dimethyl-1,3-butadiene

Measured: 4.48e-01

Predicted: 204