

N,N-Diethylaniline
91-66-7 | DTXSID8021800

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: 3.14e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.33e-01

Confidence level: 7.28e-01

Nearest Neighbors from the Training Set

Image not found

1,2-Dimethoxybenzene

Measured: 1.36e-01

Predicted: 9.15e-02

Image not found

4-Cumylphenol

Measured: 8.62e-01

Predicted: 1.23e-04

Image not found

4-Hydroxybenzoic acid

Measured: 1.78e-01

Predicted: 1.93e-06

Image not found

Triethylamine

Measured: 7.00e-01

Predicted: 36.5

Image not found

tert-Butylbenzene

Measured: 4.14e-01

Predicted: 9.58e-01