

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 12.8

Global applicability domain: Inside

Local applicability domain index: 5.54e-01

Confidence level: 6.32e-01

Nearest Neighbors from the Training Set

Image not found

Isophorone

Measured: 2.00

Predicted: 3.19

Image not found

N,N-Diethylaniline

Measured: 102

Predicted: 12.8

Image not found

Triallylamine

Measured: 3.55

Predicted: 4.23

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5-Ethylidene-2-norbornene

Measured: 110

Predicted: 134

Image not found

Menthol

Measured: 10.8

Predicted: 23.5

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(1R,2S,5R)-(-)-Menthol

Measured: 10.8

Predicted: 23.5