

N-Ethylglycine
627-01-0 | DTXSID70311675

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

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: 1.75e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.09e-01

Confidence level: 4.27e-01

Nearest Neighbors from the Training Set

Image not found

Heptacosane

Measured: 8.75e-03

Predicted: 1.05e-07

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Pentan-2-ol

Measured: 3.14e-06

Predicted: 5.03

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2-Butanethiol

Measured: 2.10e-01

Predicted: 67.6

Image not found

Diethyl carbonate

Measured: 2.00e-04

Predicted: 10.8

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2-Methylpentane

Measured: 2.01e-02

Predicted: 127