

N-Ethylglycine
627-01-0 | DTXSID70311675

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 9.73 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.27e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

Image not found

1,2-Diethylhydrazine

Measured: 15.1

Predicted: 14.1

Image not found

Diethanolamine

Measured: 3.98

Predicted: 4.00

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3-Pyridinecarbonitrile

Measured: 36.3

Predicted: 25.0

Image not found

1,4-Dioxane

Measured: 17.0

Predicted: 13.2

Image not found

1-Methoxy-2-propyl acetate

Measured: 2.29

Predicted: 7.33