

N-Methylcarbamic acid, ethyl ester
105-40-8 | DTXSID2031746

Model Performance

Model	Data
-------	------

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: 10.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.34e-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

3-Pyridinecarbonitrile

Measured: 36.3

Predicted: 25.0

Image not found

1-Methoxy-2-propyl acetate

Measured: 2.29

Predicted: 7.33

Image not found

1,4-Dioxane

Measured: 17.0

Predicted: 13.2

Image not found

Diethanolamine

Measured: 3.98

Predicted: 4.00