

Triethanolamine
102-71-6 | DTXSID9021392

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.58e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.44e-01

Confidence level: 7.87e-01

Nearest Neighbors from the Training Set

Image not found

2-(2-Butoxyethoxy)ethanol

Measured: 7.44e-11

Predicted: 5.15e-11

Image not found

1-Butoxy-2-propanol

Measured: 3.76e-11

Predicted: 3.73e-11

Image not found

2-(2-Ethoxyethoxy)ethanol

Measured: 5.72e-11

Predicted: 3.59e-11

Image not found

3-Methoxybutan-1-ol

Measured: 2.36e-11

Predicted: 2.52e-11