

Triisopropanolamine
122-20-3 | DTXSID5021415

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: 2.59e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.47e-01

Confidence level: 7.55e-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

Simazine

Measured: 1.10e-11

Predicted: 1.22e-11

Image not found

Terbutylazine

Measured: 1.10e-11

Predicted: 1.23e-11

Image not found

Butane, 1,1'-
[methylenebis(oxy)]bis-

Measured: 3.39e-11

Predicted: 3.22e-11