

1,4-Dideoxy-1,4-iminothreitol  
90481-32-6 | DTXSID50238179

## 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
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 2.74e-11 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 6.47e-01

**Confidence level:** 8.04e-01

## Nearest Neighbors from the Training Set

Image not found

2-(2-Ethoxyethoxy)ethanol

**Measured:** 5.72e-11

**Predicted:** 3.59e-11

Image not found

Diethylene glycol

**Measured:** 3.00e-11

**Predicted:** 2.21e-11

Image not found

1-Methoxy-2-propanol

**Measured:** 1.86e-11

**Predicted:** 1.93e-11

Image not found

Propane, 1,1,3-trimethoxy-

**Measured:** 1.92e-11

**Predicted:** 2.33e-11

Image not found

2-Isopropoxyethanol

**Measured:** 2.06e-11

**Predicted:** 2.11e-11