

Diethylene glycol diethyl ether
112-36-7 | DTXSID3025047

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 5.20 days

Global applicability domain: Outside

Local applicability domain index: 1.82e-01

Confidence level: 8.23e-01

Nearest Neighbors from the Training Set

Image not found

Pentane

Measured: 40.7

Predicted: 6.52

Image not found

n-Hexane

Measured: 157

Predicted: 7.45

Image not found

Heptane

Measured: 88.3

Predicted: 7.54

Image not found

Hexane, 2,2-dimethyl-

Measured: 24.3

Predicted: 4.47

Image not found

2-Methylhexane

Measured: 12.5

Predicted: 5.54