

1-Eicosanol
629-96-9 | DTXSID0027272

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.57e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.24e-01

Confidence level: 4.50e-01

Nearest Neighbors from the Training Set

Image not found

Heneicosane

Measured: 4.52e-08

Predicted: 1.71e-05

Image not found

1-Bromooctadecane

Measured: 2.70e-06

Predicted: 8.30e-06

Image not found

2-Butyne

Measured: 1.81e-09

Predicted: 797

Image not found

Octadecanoic acid

Measured: 7.22e-07

Predicted: 3.10e-07

Image not found

Diethylene glycol dibutyl ether

Measured: 1.40e-06

Predicted: 4.44e-02