

Pentaerythritol
115-77-5 | DTXSID2026943

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.20e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.79e-01

Confidence level: 4.47e-01

Nearest Neighbors from the Training Set

Image not found

Benz(a)anthracene

Measured: 1.97e-10

Predicted: 2.14e-08

Image not found

L-Glutamic acid

Measured: 1.70e-08

Predicted: 1.68e-08

Image not found

1,4-Benzenediamine, N-(2,4-dinitrophenyl)-

Measured: 3.28e-08

Predicted: 5.92e-11

Image not found

Glycerol

Measured: 1.68e-04

Predicted: 1.31e-04

Image not found

Triallylamine

Measured: 3.59e-06

Predicted: 2.91