

Benzene, 1,1'-(1,3-propanediylbis(oxy))bis-
726-44-3 | DTXSID20222924

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: 7.16e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.18e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

Image not found

2,4,5-Trichlorophenoxyacetic acid

Measured: 1.50e-05

Predicted: 4.08e-06

Image not found

Methyl benzoate

Measured: 6.16e-05

Predicted: 3.32e-01

Image not found

Fluazuron

Measured: 7.57e-05

Predicted: 1.00e-09

Image not found

Acetylugenol

Measured: 2.32e-04

Predicted: 6.51e-04

Image not found

Diphenylurea

Measured: 1.50e-04

Predicted: 1.72e-06