

Hexachloro-1,3-butadiene
87-68-3 | DTXSID7020683

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: 1.86e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.26e-01

Confidence level: 5.68e-01

Nearest Neighbors from the Training Set

Image not found

2,6-Dichlorophenol

Measured: 2.20e-01

Predicted: 1.03e-01

Image not found

Heptachlor

Measured: 6.00e-02

Predicted: 1.31e-04

Image not found

Phenyl carbonochloridate

Measured: 2.44e-01

Predicted: 1.81e-01

Image not found

Dimethyl sulfoxide

Measured: 2.10e-01

Predicted: 3.98e-01

Image not found

Methyl isothiocyanate

Measured: 2.70e-01

Predicted: 5.52