

Diethyl phosphorochloridate
814-49-3 | DTXSID4052556

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 5.71

Global applicability domain: Inside

Local applicability domain index: 9.31e-01

Confidence level: 7.27e-01

Nearest Neighbors from the Training Set

Image not found

Hexamethylbenzene

Measured: 6.31

Predicted: 5.75

Image not found

1,2,3,4-Tetrachlorobenzene

Measured: 5.64

Predicted: 5.76

Image not found

1,4-Dibromobenzene

Measured: 5.21

Predicted: 5.09

Image not found

1,2,3,5-Tetrachlorobenzene

Measured: 5.55

Predicted: 5.67

Image not found

1,2,4,5-Tetrachlorobenzene

Measured: 5.63

Predicted: 5.67