

Phosphonic acid, vinyl-, diethyl ester
682-30-4 | DTXSID70218372

Model Performance

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

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.59e-02

Global applicability domain: Inside

Local applicability domain index: 5.23e-01

Confidence level: 6.18e-01

Nearest Neighbors from the Training Set

Image not found

Diethyl ethylphosphonate

Measured: 0.66

Predicted: 6.30e-01

Image not found

Sarin

Measured: 0.3

Predicted: 3.86e-01

Image not found

Phosphonic acid, bis(1-methylethyl) ester

Measured: 0.45

Predicted: 5.25e-01

Image not found

Dimethyl (2-oxopropyl)phosphonate

Measured: -0.860

Predicted: -0.611

Image not found

Dimethyl methylphosphonate

Measured: -0.610

Predicted: -0.557