

Phosphoric acid, 2-chloroethenyl diethyl ester
311-47-7 | DTXSID3075385

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 232 °C

Global applicability domain: Inside

Local applicability domain index: 5.29e-01

Confidence level: 6.48e-01

Nearest Neighbors from the Training Set

Image not found

Dichlorvos

Measured: 234

Predicted: 221

Image not found

Sulfurous acid, bis(2-methylpropyl) ester

Measured: 210

Predicted: 214

Image not found

Cyclosarin

Measured: 239

Predicted: 216

Image not found

Sulfurous acid, dibutyl ester

Measured: 230

Predicted: 226

Image not found

Tripropyl phosphate

Measured: 252

Predicted: 244