

Diethyl phosphorochloridate  
814-49-3 | DTXSID4052556

## 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
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** -66.9 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 5.15e-01

**Confidence level:** 5.93e-01

## Nearest Neighbors from the Training Set

Image not found

Diisopropyl fluorophosphate

**Measured:** -82.0

**Predicted:** -73.2

Image not found

Sarin

**Measured:** -57.0

**Predicted:** -59.2

Image not found

Phosphonothioic acid, methyl-,  
O,o-diethyl ester

**Measured:** -84.4

**Predicted:** -62.3

Image not found

Dimethyl hydrogen phosphite

**Measured:** -60.0

**Predicted:** -61.6

Image not found

Pinacolyl  
methylphosphonofluoridate

**Measured:** -42.0

**Predicted:** -48.2