

Phosphonothioic acid, methyl-, O,o-diethyl ester
6996-81-2 | DTXSID10220237

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: 194 °C

Global applicability domain: Inside

Local applicability domain index: 5.14e-01

Confidence level: 4.89e-01

Nearest Neighbors from the Training Set

Image not found

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

Measured: 199

Predicted: 194

Image not found

Diethyl phosphorochloridate

Measured: 93.5

Predicted: 125

Image not found

Sulfurous acid, bis(2-
methylpropyl) ester

Measured: 210

Predicted: 214

Image not found

Phosphonic acid, vinyl-, diethyl
ester

Measured: 202

Predicted: 205

Image not found

Dichlorvos

Measured: 234

Predicted: 221