

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -62.3 °C

Global applicability domain: Inside

Local applicability domain index: 5.05e-01

Confidence level: 4.35e-01

Nearest Neighbors from the Training Set

Image not found

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

Measured: -84.4

Predicted: -62.3

Image not found

Ethylene glycol, cyclic sulfate

Measured: 99.0

Predicted: 56.4

Image not found

Pinacolyl
methylphosphonofluoridate

Measured: -42.0

Predicted: -48.2

Image not found

Glycol sulfite

Measured: -11.0

Predicted: -0.807

Image not found

Sarin

Measured: -57.0

Predicted: -59.2