

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

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: -64.9 °C

Global applicability domain: Inside

Local applicability domain index: 5.47e-01

Confidence level: 5.93e-01

Nearest Neighbors from the Training Set

Image not found

Pinacolyl
methylphosphonofluoridate

Measured: -42.0

Predicted: -48.2

Image not found

Diisopropyl fluorophosphate

Measured: -82.0

Predicted: -73.2

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

Triethyl phosphate

Measured: -56.4

Predicted: -54.1