

Hexamethylphosphoramide
680-31-9 | DTXSID6020694

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.86e-01

Global applicability domain: Outside

Local applicability domain index: 5.16e-01

Confidence level: 6.78e-01

Nearest Neighbors from the Training Set

Image not found

Hexamethylphosphoramide

Measured: 0.28

Predicted: 3.86e-01

Image not found

MLS003389292

Measured: 0.02

Predicted: 2.24e-01

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N,N-Diethyl-N',N',N'',N''-
tetramethylphosphoric triamide

Measured: 0.66

Predicted: 6.84e-01

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N,N,N',N'-Tetramethyl-P-
pyrrolidin-1-ylphosphonic
diamide

Measured: 0.82

Predicted: 7.91e-01