

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.56e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.72e-01

Confidence level: 6.80e-01

Nearest Neighbors from the Training Set

Image not found

Phosphoramidic acid, dimethyl-, dimethyl ester

Measured: 3.19e-11

Predicted: 2.75e-11

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Triethyl phosphate

Measured: 5.53e-11

Predicted: 4.26e-11

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O,S,S-Trimethyl phosphorodithioate

Measured: 9.59e-12

Predicted: 1.50e-11

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O,O,S- Trimethyl dithiophosphate

Measured: 5.60e-11

Predicted: 3.74e-11

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Dimefox

Measured: 6.40e-11

Predicted: 3.64e-11