

4-(Chloromethyl)-2-ethoxy-1,3,2lambda⁵- dioxaphospholan-2-one

67554-11-4 | DTXSID50791173

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: -10.5 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.98e-01

Confidence level: 7.17e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Triethyl phosphate

Measured: -10.3

Predicted: -10.4

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Phosphoramidic acid,
dimethyl-, dimethyl ester

Measured: -10.5

Predicted: -10.6

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Ethyl ethylcarbamate

Measured: -10.8

Predicted: -10.8

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N-Methylcarbamic acid,
ethyl ester

Measured: -11.1

Predicted: -11.0

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Dimefox

Measured: -10.2

Predicted: -10.4