

Diethyl phosphorochloridate  
814-49-3 | DTXSID4052556

## 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:** 2.63e-11 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 6.23e-01

**Confidence level:** 6.95e-01

## Nearest Neighbors from the Training Set

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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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Dimefox

**Measured:** 6.40e-11

**Predicted:** 3.64e-11

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O,O,S-Trimethyl phosphorothioate

**Measured:** 9.29e-12

**Predicted:** 1.56e-11

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N-Methylcarbamic acid, ethyl ester

**Measured:** 8.30e-12

**Predicted:** 1.01e-11