

# Phosphorochloridothioic acid, O,O-diethyl ester

## Other names:

Diethoxythiophosphoryl chloride  
Diethyl chlorothiophosphate  
Diethyl phosphorochloridothioate  
Diethyl phosphorochloridothionate  
Diethyl phosphorochlorothioate  
Diethyl phosphorothiochloridate  
Diethyl thiophosphoric chloride  
Diethyl thiophosphoryl chloride  
Diethylthiophosphoric acid chloride  
O,O-Diethyl chloridophosphorothioate  
O,O-Diethyl chloridothionophosphate  
O,O-Diethyl chlorothionophosphate  
O,O-Diethyl chlorothiophosphate  
O,O-Diethyl chlorothiophosphonate  
O,O-Diethyl phosphorochloridothioate  
O,O-Diethyl phosphorochlorothioate  
O,O-Diethyl phosphorothiochloridate  
O,O-Diethyl phosphorothionochloridate  
O,O-Diethyl thionophosphoric acid ester chloride  
O,O-Diethyl thionophosphoric chloride  
O,O-Diethyl thionophosphoryl chloride  
O,O-Diethyl thiophosphorochloridate  
O,O-Diethyl thiophosphoryl chloride  
O,O-Diethyl thiophosphoric acid chloride  
Diethyl phosphorothionochloridate  
Diethylchlorthiofosfat  
Ethyl pct  
O,O-Diethyl thionophosphorochloridate  
O,O-Diethylester kyseliny chlorthiofosforecne  
Phosphonothioic acid, chloro-, O,O-diethyl ester  
UN 2751  
O,O-Diethylchlorothiophosphidate  
NSC 43776  
Phosphorochloridothioic acid, o,o'-diethyl ester

**Inchi:** InChI=1S/C4H10ClO2PS/c1-3-6-8(5,9)7-4-2/h3-4H2,1-2H3  
**InchiKey:** KMJJTCKNZYTEY-UHFFFAOYSA-N  
**Formula:** C4H10ClO2PS  
**SMILES:** CCOP(=S)(Cl)OCC  
**Mol. weight [g/mol]:** 188.61  
**CAS:** 2524-04-1

# Physical Properties

Property code	Value	Unit	Source
ie	8.80	eV	NIST Webbook
ie	8.83 ± 0.02	eV	NIST Webbook
ie	9.31	eV	NIST Webbook
ie	9.41	eV	NIST Webbook
ie	9.41	eV	NIST Webbook
log10ws	1.92		Crippen Method
logp	2.523		Crippen Method
mcvol	128.010	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2524041&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2524041&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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