Phosphorochloridic acid, diethyl ester

Other names:	Diethoxyphosphorus oxychloride Diethoxyphosphoryl chloride Diethyl chlorophosphate Diethyl phosphorochloridate Diethyl phosphorochloride Diethylphosphoric acid chloride Ethyl phosphorochloridate (Cl(EtO)2PO) Ethyl phosphorochloridate (EtO)2ClPO O,O-Diethyl chloridophosphate O,O-Diethyl chlorophosphate O,O-Diethyl chlorophosphonate O,O-Diethyl phosphorochloridate O,O-Diethylphosphoryl chloride Phosphine oxide, chlorodiethoxy- Chlorophosphoric acid, diethyl ester Diethyl chlorophosphonate Diethylchlorfosfat Ethyl phosphorochloridate Chlorodiethoxyphosphine oxide Chlorodiethylphosphate Diethyl phosphochloridate NSC 43770
Inchi:	InChI=1S/C4H10ClO3P/c1-3-7-9(5,6)8-4-2/h3-4H2,1-2H3
InchiKey:	LGTLXDJOAJDFLR-UHFFFAOYSA-N
Formula:	C4H10ClO3P
SMILES:	CCOP(=O)(Cl)OCC
Mol. weight [g/mol]:	172.55
CAS:	814-49-3

Physical Properties

Property code	Value	Unit	Source
ie	10.40	eV	NIST Webbook
ie	10.29	eV	NIST Webbook
ie	11.07	eV	NIST Webbook
log10ws	-3.09		Crippen Method
logp	2.406		Crippen Method

mcvol	117.530	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C814493&Units=SI

Legend

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

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