

Phosphorodichloridic acid, propyl ester

Inchi:	InChI=1S/C3H7Cl2O2P/c1-2-3-7-8(4,5)6/h2-3H2,1H3
InchiKey:	YTXISYSGCBTCGY-UHFFFAOYSA-N
Formula:	C3H7Cl2O2P
SMILES:	CCCOP(=O)(Cl)Cl
Mol. weight [g/mol]:	176.97
CAS:	10173-43-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	2.999		Crippen Method
mcvol	109.810	ml/mol	McGowan Method

Sources

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=C10173430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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