

Phosphonic acid, chloromethyl-, p-chlorophenyl ethyl ester

Inchi:	InChI=1S/C9H11Cl2O3P/c1-2-13-15(12,7-10)14-9-5-3-8(11)4-6-9/h3-6H,2,7H2,1H3
InchiKey:	BHUNCGBHHYHPJG-UHFFFAOYSA-N
Formula:	C9H11Cl2O3P
SMILES:	CCOP(=O)(CCl)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	269.06
CAS:	116401-61-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	4.145		Crippen Method
mcvol	176.460	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116401617&Units=SI

Legend

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

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