

Phosphonic acid, chloromethyl-, bis(4-chlorophenyl) ester

Inchi:	InChI=1S/C13H10Cl3O3P/c14-9-20(17,18-12-5-1-10(15)2-6-12)19-13-7-3-11(16)4-8-13/
InchiKey:	BCJSMEBHAUEMOB-UHFFFAOYSA-N
Formula:	C13H10Cl3O3P
SMILES:	O=P(CCl)(Oc1ccc(Cl)cc1)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	351.55
CAS:	66392-83-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.23		Crippen Method
logp	5.841		Crippen Method
mcvol	221.300	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=C66392834&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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