

Phosphonic acid, chloromethyl-, bis(2-chlorophenyl) ester

Inchi:	InChI=1S/C13H10Cl3O3P/c14-9-20(17,18-12-7-3-1-5-10(12)15)19-13-8-4-2-6-11(13)16/
InchiKey:	PONSXOVORYEUNA-UHFFFAOYSA-N
Formula:	C13H10Cl3O3P
SMILES:	O=P(CCl)(Oc1ccccc1Cl)Oc1ccccc1Cl
Mol. weight [g/mol]:	351.55
CAS:	105972-87-0

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105972870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/122-966-4/Phosphonic-acid-chloromethyl-bis-2-chlorophenyl-ester.pdf>

Generated by Cheméo on 2024-04-30 04:21:50.4444070005 +0000 UTC m=+16740159.364647320.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.