2,4,5-Trichlorophenyl dichloridophosphate

Inchi:	InChI=1S/C6H2Cl5O2P/c7-3-1-5(9)6(2-4(3)8)13-14(10,11)12/h1-2H
InchiKey:	BWCWBOSYZRQRDR-UHFFFAOYSA-N
Formula:	C6H2Cl5O2P
SMILES:	O=P(Cl)(Cl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	314.32
CAS:	2213-71-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.80		Crippen Method
logp	5.611		Crippen Method
mcvol	165.040	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2213710&Units=SI
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

Legend

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

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