O-(2,4,5-trichlorophenyl) dichloridothiophosphate

Inchi: InChI=1S/C6H2Cl5OPS/c7-3-1-5(9)6(2-4(3)8)12-13(10,11)14/h1-2H
InchiKey: NLMYUXLTZXZAJR-UHFFFAOYSA-N
Formula: C6H2Cl5OPS
SMILES: S=P(Cl)(Cl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 330.38
CAS: 16805-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	5.728		Crippen Method
mcvol	175.520	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=C16805780&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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