Phosphoramidic acid, (2,4,5-trichlorophenyl) ethyl ester

Inchi: InChI=1S/C8H9Cl3NO3P/c1-2-14-16(12,13)15-8-4-6(10)5(9)3-7(8)11/h3-4H,2H2,1H3,(H
InchiKey: CGANBZPQXLOTHR-UHFFFAOYSA-N
Formula: C8H9Cl3NO3P
SMILES: CCOP(N)(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 304.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	4.129		Crippen Method
mcvol	184.590	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=B6001021&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