O-methyl o-(2,4,5-trichlorophenyl) amidothiophosphate

Inchi: InChI=1S/C7H7Cl3NO2PS/c1-12-14(11,15)13-7-3-5(9)4(8)2-6(7)10/h2-3H,1H3,(H2,11,15

InchiKey: WRWBHVIYUCQSIA-UHFFFAOYSA-N

Formula: C7H7Cl3NO2PS

SMILES: COP(N)(=S)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 306.53

CAS: 2591-66-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.42		Crippen Method
logp	3.855		Crippen Method
mcvol	180.980	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2591664&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume