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

Inchi: InChI=1S/C8H9Cl3NO2PS/c1-12-15(16,13-2)14-8-4-6(10)5(9)3-7(8)11/h3-4H,1-2H3,(H,1

InchiKey: HCLXTCZCKDQWDL-UHFFFAOYSA-N

Formula: C8H9Cl3NO2PS

SMILES: CNP(=S)(OC)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 320.56

CAS: 2591-70-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	4.116		Crippen Method
mcvol	195.070	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2591700&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