O-methyl,o-(2,4,5-trichlorophenyl)n-ethyl phosphoramidothioate

Inchi: InChI=1S/C9H11Cl3NO2PS/c1-3-13-16(17,14-2)15-9-5-7(11)6(10)4-8(9)12/h4-5H,3H2,1

InchiKey: FHADYQBDCIGGEE-UHFFFAOYSA-N

Formula: C9H11Cl3NO2PS

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

Mol. weight [g/mol]: 334.59

CAS: 2591-74-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	4.506		Crippen Method
mcvol	209.160	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=C2591744&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume