O-(2,4,5-trichlorophenyl) n,n'-diphenyldiamidothiophosphate

Inchi: InChI=1S/C18H14Cl3N2OPS/c19-15-11-17(21)18(12-16(15)20)24-25(26,22-13-7-3-1-4-8

InchiKey: MBPRWSAZMWODKG-UHFFFAOYSA-N

Formula: C18H14Cl3N2OPS

SMILES: S=P(Nc1ccccc1)(Nc1ccccc1)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 443.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	7.474		Crippen Method
mcvol	292.560	ml/mol	McGowan Method

Sources

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=B6009199&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume