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

Inchi: InChI=1S/C10H14Cl3N2OPS/c1-3-14-17(18,15-4-2)16-10-6-8(12)7(11)5-9(10)13/h5-6H,3

InchiKey: LSUSXIYJONKJAQ-UHFFFAOYSA-N

Formula: C10H14Cl3N2OPS

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

Mol. weight [g/mol]: 347.63

CAS: 110252-31-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Crippen Method
logp	4.469		Crippen Method
mcvol	227.360	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=C110252318&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume