

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

Inchi: InChI=1S/C10H14Cl3N2OPS/c1-14(2)17(18,15(3)4)16-10-6-8(12)7(11)5-9(10)13/h5-6H,
InchiKey: INPRLIDPDDNKEY-UHFFFAOYSA-N
Formula: C10H14Cl3N2OPS
SMILES: CN(C)P(=S)(Oc1cc(Cl)c(Cl)cc1Cl)N(C)C
Mol. weight [g/mol]: 347.63
CAS: 110252-33-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.30		Crippen Method
logp	4.373		Crippen Method
mcvol	227.360	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=C110252330&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

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