

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

Inchi: InChI=1S/C8H10Cl3N2OPS/c1-12-15(16,13-2)14-8-4-6(10)5(9)3-7(8)11/h3-4H,1-2H3,(H,1-2H3)
InchiKey: WAHJDCHWLCLNBQ-UHFFFAOYSA-N
Formula: C8H10Cl3N2OPS
SMILES: CNP(=S)(NC)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 319.58
CAS: 16805-77-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.70		Crippen Method
logp	3.689		Crippen Method
mcvol	199.180	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=C16805779&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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