

O-methyl-o-(2,4,5-trichlorophenyl)chlorothiophosphate

Inchi: InChI=1S/C7H5Cl4O2PS/c1-12-14(11,15)13-7-3-5(9)4(8)2-6(7)10/h2-3H,1H3
InchiKey: WCJAXYHKRXTTIH-UHFFFAOYSA-N
Formula: C7H5Cl4O2PS
SMILES: COP(=S)(Cl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 325.96
CAS: 948-95-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.14		Crippen Method
logp	5.135		Crippen Method
mcvol	183.240	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=C948958&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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<https://www.chemeo.com/cid/67-053-9/O-methyl-o-2-4-5-trichlorophenyl-chlorothiophosphate.pdf>

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