

O-methyl o,o-bis(2,4,5-trichlorophenyl) thiophosphate

Inchi: InChI=1S/C13H7Cl6O3PS/c1-20-23(24,21-12-4-8(16)6(14)2-10(12)18)22-13-5-9(17)7(15)
InchiKey: ACVLAMDDCNEKCJ-UHFFFAOYSA-N
Formula: C13H7Cl6O3PS
SMILES: COP(=S)(Oc1cc(Cl)c(Cl)cc1Cl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 486.95
CAS: 56201-37-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	7.936		Crippen Method
mcvol	274.370	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56201377&Units=SI>
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>

Legend

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

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