

O-propyl o-(2,4,5-trichlorophenyl)amidothiophosphate

Inchi:	InChI=1S/C9H11Cl3NO2PS/c1-2-3-14-16(13,17)15-9-5-7(11)6(10)4-8(9)12/h4-5H,2-3H2
InchiKey:	YXRPPALJUAKPHT-UHFFFAOYSA-N
Formula:	C9H11Cl3NO2PS
SMILES:	CCCOP(N)(=S)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	334.59
CAS:	2591-67-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.26		Crippen Method
logp	4.635		Crippen Method
mcvol	209.160	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=C2591675&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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