

Phosphoramidothioic acid, o-ethyl-o-(2,4,5-trichlorophenyl) ester

Inchi:	InChI=1S/C8H9Cl3NO2PS/c1-2-13-15(12,16)14-8-4-6(10)5(9)3-7(8)11/h3-4H,2H2,1H3,(
InchiKey:	WNKUETVZFUAQCI-UHFFFAOYSA-N
Formula:	C8H9Cl3NO2PS
SMILES:	CCOP(N)(=S)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	320.56
CAS:	2775-95-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	4.245		Crippen Method
mcvol	195.070	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2775953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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