

O-butyl, o-(2,4,5-trichlorophenyl)phosphor amidothioate

Inchi:	InChI=1S/C10H13Cl3NO2PS/c1-2-3-4-15-17(14,18)16-10-6-8(12)7(11)5-9(10)13/h5-6H,1
InchiKey:	KFHRJFSDWFWPGE-UHFFFAOYSA-N
Formula:	C10H13Cl3NO2PS
SMILES:	CCCCOP(N)(=S)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	348.61
CAS:	2591-68-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	5.026		Crippen Method
mcvol	223.250	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=C2591686&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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