

O-ethyl-o-(2,4,6-trichlorophenyl)-n-ethylamido thiophosphate

Inchi:	InChI=1S/C10H13Cl3NO2PS/c1-3-14-17(18,15-4-2)16-10-8(12)5-7(11)6-9(10)13/h5-6H,
InchiKey:	ONQYCWOFIFYCJG-UHFFFAOYSA-N
Formula:	C10H13Cl3NO2PS
SMILES:	CCNP(=S)(OCC)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	348.61
CAS:	116401-94-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	4.896		Crippen Method
mcvol	223.250	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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