

Tolclofos-methyl

Other names:	Phosphorothioic acid, O-(2,6-dichloro-4-methylphenyl) O,O-dimethyl ester Basilex Dimethyl O-(2,6-dichloro-4-methylphenyl) phosphorothioate O-(2,6-Dichloro-4-methylphenyl) O,O-dimethyl phosphorothioate Risolet Rizolex S-3349 Tolclofos-methyl O,O-Dimethyl O-(2,6-dichloro-4-methylphenyl) phosphorothioate O-(2,6-dichloro-p-tolyl) O,O-dimethyl thiophosphate
Inchi:	InChI=1S/C9H11Cl2O3PS/c1-6-4-7(10)9(8(11)5-6)14-15(16,12-2)13-3/h4-5H,1-3H3
InchiKey:	OBZIQQJJIKNWNQ-UHFFFAOYSA-N
Formula:	C9H11Cl2O3PS
SMILES:	COP(=S)(OC)Oc1c(Cl)cc(C)cc1Cl
Mol. weight [g/mol]:	301.13
CAS:	57018-04-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.28		Crippen Method
logp	4.198		Crippen Method
mcvol	192.810	ml/mol	McGowan Method
rinpol	1861.00		NIST Webbook
rinpol	1882.00		NIST Webbook
rinpol	1899.00		NIST Webbook
rinpol	1861.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57018049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices

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