Bromophos-ethyl

Other names:	Phosphorothioic acid, O-(4-bromo-2,5-dichlorophenyl) O,O-diethyl ester
	Ethyl Bromophos
	Filariol 60
	Nexagan G
	OMS 659
	O-(4-Bromo-2,5 dichlorophenyl) OO-diethyl phosphorothioate
	O-(4-Bromo-2,5 dichlorophenyl) O,O-diethylphosphorothionate
	Bromofos-ethyl
	CELA S-2225
	O,O-Diaethyl-O-(4-brom-2,5-dichlor)-phenyl-monothiophosphat
	O,O-Diaethyl-O-(2,5-dichlor-4-bromphenyl)-thionophosphat
	O,O-Diethyl-O-(4-broom-2,5-dichloor-fenyl)-monothiofosfaat
	O,O-Diethyl O-(2,5-dichloro-4-bromophenyl) thiophosphate
	O,O-Diethyl O-2,5-dichloro-4-bromophenyl-phosphorothioate
	O,O-Dietil-O-(4-bromo-2,5 dicloro-fenil)-monotiofosfato
	ENT 27,258
	Filariol
	Nexagan
	Phenol, 4-bromo-2,5-dichloro-, O-ester with O,O-diethyl phosphorothioate
	S 2225
	Thiophosphate de O,O-diethyle et de O-(2,5-dichloro-4-bromo) phenyle
Inchi:	InChI=1S/C10H12BrCl2O3PS/c1-3-14-17(18,15-4-2)16-10-6-8(12)7(11)5-9(10)13/h5-6H,
InchiKey:	KWGUFOITWDSNQY-UHFFFAOYSA-N
Formula:	C10H12BrCl2O3PS
SMILES:	CCOP(=S)(OCC)Oc1cc(Cl)c(Br)cc1Cl
Mol. weight [g/mol]:	394.05
CAS:	4824-78-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Crippen Method
logp	5.432		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
rinpol	2105.00		NIST Webbook

rinpol	2134.00	NIST Webbook
rinpol	2135.00	NIST Webbook
rinpol	2075.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4824786&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices