Profenofos

Other names:	Phosphorothioic acid, O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl ester
	Profenophos
	Polycron
	Curacron
	Selecron
	O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl phosphorothioate
Inchi:	InChI=1S/C11H15BrClO3PS/c1-3-7-18-17(14,15-4-2)16-11-6-5-9(12)8-10(11)13/h5-6,8H
InchiKey:	QYMMJNLHFKGANY-UHFFFAOYSA-N
Formula:	C11H15BrClO3PS
SMILES:	CCCSP(=O)(OCC)Oc1ccc(Br)cc1Cl
Mol. weight [g/mol]:	373.63
CAS:	41198-08-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.35		Crippen Method
logp	5.769		Crippen Method
mcvol	226.250	ml/mol	McGowan Method
rinpol	2165.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2186.00		NIST Webbook

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=C41198087&Units=SI

Legend

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