Leptophos

Other names:	(.+/-.)-Leptophos
	Abar
	Fosvel
	K62-105
	MBCP
	NK 711
	O-(2,5-Dichloro-4-bromophenyl) O-methyl phenylthiophosphonate
	O-(4-Bromo-2,5-Dichlorophenyl) O-methyl phenylphosphonothioate
	O-Methyl O-2,5-dichloro-4-bromophenyl phenylthiophosphonate
	O-Methyl-O-(4-bromo-2,5-dichlorophenyl)phenyl thiophosphonate
	OMS 1438
	Oleophosvel
	Phenylphosphonothioic acid O-(4-bromo-2,5-dichlorophenyl) O-methyl ester
	Phosphonothioic acid, phenyl-, O-(4-bromo-2,5-dichlorophenyl) O-methyl ester
	Phosvel
	VCS 506
	Velsicol 506
	Velsicol VCS 506
Inchi:	InChI=1S/C13H10BrCl2O2PS/c1-17-19(20,9-5-3-2-4-6-9)18-13-8-11(15)10(14)7-12(13)1
InchiKey:	CVRALZAYCYJELZ-UHFFFAOYSA-N
Formula:	C13H10BrCl2O2PS
SMILES:	COP(=S)(Oc1cc(Cl)c(Br)cc1Cl)c1ccccc1
Mol. weight [g/mol]:	412.07
CAS:	21609-90-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.66		Aqueous Solubility Prediction Method
logp	5.416		Crippen Method
mcvol	237.040	ml/mol	McGowan Method
rinpol	2495.00		NIST Webbook
rinpol	2486.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2486.00		NIST Webbook
tf	343.55	K	Aqueous Solubility Prediction Method

tf	347.14 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	31.35	kJ/mol	345.60	NIST Webbook
hfust	31.35	kJ/mol	345.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21609905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point