o-(4-Bromo-2,5-dichlorophenyl) o-methyl phenylphosphonothioate

Other names: (.+/-.)-Leptophos
Abar
Fosvel
K62-105
MBCP
NK 711
O-(2,5-Dichloro-4-bromophenyl) O-methyl phenylthiophosphonate
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
leptophos

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

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

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21609905&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

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