

Leptophos oxon

Other names:	Phosphonic acid, phenyl-, 4-bromo-2,5-dichlorophenyl methyl ester Phosvel oxon Velsicol VCS-506 O-analog Leptophos OA Leptophos oxygen analog Phenylphosphonic acid 4-bromo-2,5-dichlorophenyl methyl ester Leptophoxon
Inchi:	InChI=1S/C13H10BrCl2O3P/c1-18-20(17,9-5-3-2-4-6-9)19-13-8-11(15)10(14)7-12(13)16
InchiKey:	MAKU YRKZFGSMMG-UHFFFAOYSA-N
Formula:	C13H10BrCl2O3P
SMILES:	COP(=O)(Oc1cc(Cl)c(Br)cc1Cl)c1ccccc1
Mol. weight [g/mol]:	396.00
CAS:	25006-32-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.49		Crippen Method
logp	5.300		Crippen Method
mccvol	226.560	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25006320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/19-793-1/Leptophos-oxon.pdf>

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