

Shell sd-8280

Other names: (Z)-Dimethylvinphos
Inchi: InChI=1S/C10H10Cl3O4P/c1-15-18(14,16-2)17-10(6-11)8-4-3-7(12)5-9(8)13/h3-6H,1-2H
InchiKey: QSGNQELHULIMSJ-POHAHGRESA-N
Formula: C10H10Cl3O4P
SMILES: COP(=O)(OC)OC(=CCl)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 331.52
CAS: 109202-92-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.17		Crippen Method
logp	4.948		Crippen Method
mcvol	204.360	ml/mol	McGowan Method
rinsol	1986.00		NIST Webbook
rinsol	1986.00		NIST Webbook

Sources

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=C109202928&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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