

Dimethyl 3-chlorophenyl phosphate

Inchi: InChI=1S/C8H10ClO4P/c1-11-14(10,12-2)13-8-5-3-4-7(9)6-8/h3-6H,1-2H3
InchiKey: VOGWYEXFVKYZRR-UHFFFAOYSA-N
Formula: C8H10ClO4P
SMILES: COP(=O)(OC)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 236.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	3.120		Crippen Method
mcvol	156.000	ml/mol	McGowan Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2300.00		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=R168979&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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