

Diethyl 4-chlorophenyl phosphate

Inchi: InChI=1S/C10H14ClO4P/c1-3-13-16(12,14-4-2)15-10-7-5-9(11)6-8-10/h5-8H,3-4H2,1-2H
InchiKey: LBGVKIMCKGXEEF-UHFFFAOYSA-N
Formula: C10H14ClO4P
SMILES: CCOP(=O)(OCC)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 264.64
CAS: 5076-63-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	3.900		Crippen Method
mcvol	184.180	ml/mol	McGowan Method
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
ripol	2410.00		NIST Webbook
ripol	2410.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5076631&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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