

Diethyl 4-cyano-phenyl phosphate

Inchi: InChI=1S/C11H14NO4P/c1-3-14-17(13,15-4-2)16-11-7-5-10(9-12)6-8-11/h5-8H,3-4H2,1-2H3
InchiKey: PHEAVLINHUOYPR-UHFFFAOYSA-N
Formula: C11H14NO4P
SMILES: CCOP(=O)(OCC)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 255.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	3.118		Crippen Method
mcvol	187.410	ml/mol	McGowan Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
ripol	2762.00		NIST Webbook
ripol	2762.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R168959&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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