Dimethyl 3-cyano-phenyl phosphate

Inchi: InChI=1S/C9H10NO4P/c1-12-15(11,13-2)14-9-5-3-4-8(6-9)7-10/h3-6H,1-2H3
InchiKey: KAOVBKCOGJNYGW-UHFFFAOYSA-N
Formula: C9H10NO4P
SMILES: COP(=O)(OC)Oc1cccc(C#N)c1
Mol. weight [g/mol]: 227.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	2.338		Crippen Method
mcvol	159.230	ml/mol	McGowan Method
rinpol	1678.00		NIST Webbook
ripol	2625.00		NIST Webbook
ripol	2625.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R168984&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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