Pentyl N,N-dimethylphosphoramidocyanidate

Inchi: InChI=1S/C8H17N2O2P/c1-4-5-6-7-12-13(11,8-9)10(2)3/h4-7H2,1-3H3
InchiKey: KRZMSMZGUOEPSX-UHFFFAOYSA-N
Formula: C8H17N2O2P
SMILES: CCCCCOP(=O)(C#N)N(C)C
Mol. weight [g/mol]: 204.21
CAS: 148461-87-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.429		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
rinpol	1412.00		NIST Webbook
rinpol	1411.80		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1411.80		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C148461874&Units=SI

Legend

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