Propyl N,N-dimethylphosphoramidocyanidate

Inchi: InChI=1S/C6H13N2O2P/c1-4-5-10-11(9,6-7)8(2)3/h4-5H2,1-3H3
InchiKey: ZRUXFIZQYXRBHS-UHFFFAOYSA-N
Formula: C6H13N2O2P
SMILES: CCCOP(=O)(C#N)N(C)C
Mol. weight [g/mol]: 176.15
CAS: 162085-86-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	1.649		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
rinpol	1222.00		NIST Webbook
rinpol	1222.10		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1222.10		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C162085861&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