Heptyl N,N-dimethylphosphoramidocyanidate

Inchi: InChI=1S/C10H21N2O2P/c1-4-5-6-7-8-9-14-15(13,10-11)12(2)3/h4-9H2,1-3H3
InchiKey: IULLXAGGNGNYCT-UHFFFAOYSA-N
Formula: C10H21N2O2P
SMILES: CCCCCCCOP(=O)(C#N)N(C)C
Mol. weight [g/mol]: 232.26
CAS: 162085-91-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	3.209		Crippen Method
mcvol	195.320	ml/mol	McGowan Method
rinpol	1610.90		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1610.90		NIST Webbook
rinpol	1611.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C162085918&Units=SI
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

Legend

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

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