

s-Butyl N,N-dimethylphosphoramidocyanidate

Other names: Sec-butyl N,N-dimethylphosphoramidocyanidate
Inchi: InChI=1S/C7H15N2O2P/c1-5-7(2)11-12(10,6-8)9(3)4/h7H,5H2,1-4H3
InchiKey: MNNZKDXMTXPOGG-UHFFFAOYSA-N
Formula: C7H15N2O2P
SMILES: CCC(C)OP(=O)(C#N)N(C)C
Mol. weight [g/mol]: 190.18
CAS: 162085-89-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.037		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
rinpol	1256.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1259.30		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1259.30		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=C162085894&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

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