

Isobutyl N,N-dimethylphosphoramidocyanidate

Inchi: InChI=1S/C7H15N2O2P/c1-7(2)5-11-12(10,6-8)9(3)4/h7H,5H2,1-4H3
InchiKey: ABOMIXJSAGGIRO-UHFFFAOYSA-N
Formula: C7H15N2O2P
SMILES: CC(C)COP(=O)(C#N)N(C)C
Mol. weight [g/mol]: 190.18
CAS: 162085-88-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	1.895		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
rinpol	1273.00		NIST Webbook
rinpol	1279.90		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1273.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C162085883&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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