

# Phosphoramidocyanidic acid, N,N-dimethyl-, isopropyl ester

<b>Other names:</b>	Dimethylamido-isopropoxy-phosphoryl cyanide Isopropyl-N-dimethyl phosphoramidocyanidate Isopropyl N,N-dimethylphosphoramidocyanidate
<b>Inchi:</b>	InChI=1S/C6H13N2O2P/c1-6(2)10-11(9,5-7)8(3)4/h6H,1-4H3
<b>InchiKey:</b>	UQPMVHZOZHVLJ-UHFFFAOYSA-N
<b>Formula:</b>	C6H13N2O2P
<b>SMILES:</b>	CC(C)OP(=O)(C#N)N(C)C
<b>Mol. weight [g/mol]:</b>	176.15
<b>CAS:</b>	63815-55-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	1.647		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
rinpol	1161.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1161.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C63815554&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C63815554&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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