

4-(Delta'-cyclohexenyl)-1-methyl-isonipecotonitril

Inchi:	InChI=1S/C13H20N2/c1-15-9-7-13(11-14,8-10-15)12-5-3-2-4-6-12/h5H,2-4,6-10H2,1H3
InchiKey:	AFILBIDLBQNROT-UHFFFAOYSA-N
Formula:	C13H20N2
SMILES:	CN1CCC(C#N)(C2=CCCCC2)CC1
Mol. weight [g/mol]:	204.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	2.722		Crippen Method
mcvol	179.370	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000672&Units=SI
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

Legend

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

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