

# 2-[2-Hydroxy-3-(N-methyl-2-pyrrolidinyl)propanyl]pyrrolidine (isomer 2)

InChI: InChI=1S/C13H26N2O/c1-14-7-3-5-11(14)9-13(16)10-12-6-4-8-15(12)2/h11-13,16H,3-10H2  
InChIKey: UOJNOOLFFFFKNA-UHFFFAOYSA-N  
Formula: C13H26N2O  
SMILES: CN1CCCC1CC(O)CC1CCCN1C  
Mol. weight [g/mol]: 226.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	1.316		Crippen Method
mcvol	198.140	ml/mol	McGowan Method
rinpol	1695.00		NIST Webbook
rinpol	1695.00		NIST Webbook

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R573183&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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