2-[2-Hydroxy-3-(N-methyl-2-pyrrolidinyl)propanyl] (isomer 1)

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,3-10

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	1682.00		NIST Webbook
rinpol	1682.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R573178&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.