tropan-3«beta»-ol

Inchi: InChI=1S/C8H15NO/c1-9-6-2-3-7(9)5-8(10)4-6/h6-8,10H,2-5H2,1H3/t6-,7+,8-
InchiKey: CYHOMWAPJJPNMW-RNLVFQAGSA-N
Formula: C8H15NO
SMILES: CN1C2CCC1CC(O)C2
Mol. weight [g/mol]: 141.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.13		Crippen Method
logp	0.604		Crippen Method
mcvol	117.710	ml/mol	McGowan Method
rinpol	1187.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R510211&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