7«beta»-Hydroxy-1-methylene-8«alpha»/«beta»-py

Inchi: InChI=1S/C8H13NO/c1-6-2-4-9-5-3-7(10)8(6)9/h7-8,10H,1-5H2/t7-,8?/m0/s1
InchiKey: OVTJHGIWYOOHFS-JAMMHHFISA-N
Formula: C8H13NO
SMILES: C=C1CCN2CCC(O)C12
Mol. weight [g/mol]: 139.19

Physical Properties

Property code	Value	Unit	Source
logp	0.382		Crippen Method
mcvol	113.410	ml/mol	McGowan Method
rinpol	1170.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1170.00		NIST Webbook

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R590188&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices