7«alpha»-Hydroxy-1-methoxymethyl-8«alpha»-pyr

Inchi: InChI=1S/C9H17NO2/c1-12-6-7-2-4-10-5-3-8(11)9(7)10/h7-9,11H,2-6H2,1H3/t7?,8-,9+/m
InchiKey: SOCHNDUJXVADAC-ASODMVGOSA-N
Formula: C9H17NO2
SMILES: COCC1CCN2CCC(O)C12
Mol. weight [g/mol]: 171.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.28		Crippen Method
logp	0.088		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
rinpol	1422.00		NIST Webbook
rinpol	1422.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: 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=R590222&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

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