

3,6-Dihydroxytropane

Inchi: InChI=1S/C8H15NO2/c1-9-5-2-6(10)4-7(9)8(11)3-5/h5-8,10-11H,2-4H2,1H3/t5-,6?,7+,8?
InchiKey: QWVUOVZJBNQSNS-AEMDVCDZSA-N
Formula: C8H15NO2
SMILES: CN1C2CC(O)CC1C(O)C2
Mol. weight [g/mol]: 157.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.51		Crippen Method
logp	-0.425		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
rinpol	1329.00		NIST Webbook
rinpol	1329.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R421364&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

Latest version available from:

<https://www.chemeo.com/cid/54-465-6/3-6-Dihydroxytropane.pdf>

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