8-Azabicyclo[3.2.1]octane-3,6-diol, 8-methyl-, 3-acetate

Other names: 3-Acetoxy-6-hydroxytropane
Inchi: InChI=1S/C10H17NO3/c1-6(12)14-8-3-7-4-10(13)9(5-8)11(7)2/h7-10,13H,3-5H2,1-2H3
InchiKey: IQJHMKLTWPJIHO-UHFFFAOYSA-N
Formula: C10H17NO3
SMILES: CC(=O)OC1CC2CC(O)C(C1)N2C
Mol. weight [g/mol]: 199.25
CAS: 54725-46-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Crippen Method
logp	0.146		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54725461&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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