8-Azabicyclo[3.2.1]octane-3,6-diol, diacetate (ester)

Other names: 3,6-Diacetoxytropane
Inchi: InChI=1S/C12H19NO4/c1-7(14)16-10-4-9-5-12(17-8(2)15)11(6-10)13(9)3/h9-12H,4-6H2,
InchiKey: ZBNGGJNWFWYOJK-UHFFFAOYSA-N
Formula: C12H19NO4
SMILES: CC(=O)OC1CC2CC(OC(C)=O)C(C1)N2C
Mol. weight [g/mol]: 241.28
CAS: 20399-48-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	0.716		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
rinpol	1689.00		NIST Webbook
rinpol	1636.00		NIST Webbook

Sources

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=C20399488&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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