

3-(Hydroxyisovaleroxy)tropane

Inchi: InChI=1S/C13H23NO3/c1-13(2,16)8-12(15)17-11-6-9-4-5-10(7-11)14(9)3/h9-11,16H,4-8
InchiKey: IIOAFINUGUGFFZ-ZACCUICWSA-N
Formula: C13H23NO3
SMILES: CN1C2CCC1CC(OC(=O)CC(C)(C)O)C2
Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	1.316		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
rinpol	1669.00		NIST Webbook
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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=R509825&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

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<https://www.chemeo.com/cid/59-352-6/3-Hydroxyisovaleroxy-tropane.pdf>

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