

3-Isobutyryloxy-6-hydroxytropane

Inchi: InChI=1S/C12H21NO3/c1-7(2)12(15)16-9-4-8-5-11(14)10(6-9)13(8)3/h7-11,14H,4-6H2,1
InchiKey: CURGAJAGSGATLQ-QPBDYMMBSA-N
Formula: C12H21NO3
SMILES: CC(C)C(=O)OC1CC2CC(O)C(C1)N2C
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	0.782		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
rinpol	1570.00		NIST Webbook
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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=R421611&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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<https://www.chemeo.com/cid/38-440-1/3-Isobutyryloxy-6-hydroxytropane.pdf>

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