

3-Isovaleryloxy-6-hydroxytropane

Inchi: InChI=1S/C13H23NO3/c1-8(2)4-13(16)17-10-5-9-6-12(15)11(7-10)14(9)3/h8-12,15H,4-7
InchiKey: APLLVFVOTXZBFO-UZEXVOJHSA-N
Formula: C13H23NO3
SMILES: CC(C)CC(=O)OC1CC2CC(O)C(C1)N2C
Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	1.172		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
rinsol	1665.00		NIST Webbook
rinsol	1665.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R421626&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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