

3-Hydroxy-6-methylbutyryloxytropane

Other names:	3-Hydroxy-6-(2-methylbutyryloxy)-tropane
Inchi:	InChI=1S/C13H23NO3/c1-4-8(2)13(16)17-12-6-9-5-10(15)7-11(12)14(9)3/h8-12,15H,4-7
InchiKey:	ISEGEIWRXCOCGD-UHFFFAOYSA-N
Formula:	C13H23NO3
SMILES:	CCC(C)C(=O)OC1CC2CC(O)CC1N2C
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
rinpol	1675.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1725.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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