3«alpha»-(2-Methylbutyroxy)tropane

Inchi: InChI=1S/C13H23NO2/c1-4-9(2)13(15)16-12-7-10-5-6-11(8-12)14(10)3/h9-12H,4-8H2,1-
InchiKey: OGQXAZJUVVPCRL-KVMUQPTRSA-N
Formula: C13H23NO2
SMILES: CCC(C)C(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]: 225.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	2.201		Crippen Method
mcvol	189.730	ml/mol	McGowan Method
rinpol	1547.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R509523&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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