6-(2-Methylbutyroxy)-tropan-3-ol

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
CAS: 110024-54-9

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	1798.40		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1798.40		NIST Webbook
rinpol	1730.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C110024549&Units=SI
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

Legend

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