Amabiline

Inchi: InChI=1S/C16H27NO4/c1-10(2)16(20,11(3)18)12(4)21-9-13-5-7-17-8-6-14(19)15(13)17/h
InchiKey: LCGFFVMHSUIPAC-OLSVDGPUSA-N
Formula: C16H27NO4
SMILES: C=C(OCC1=CCN2CCC(O)C12)C(O)(C(C)C)C(C)O
Mol. weight [g/mol]: 297.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	0.660		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook

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=R178377&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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