

[(3R)-7-Hydroxy-8-methyl-8-azabicyclo[3.2.1]octan-3-yl)-(E)-3-methylpent-2-enoate

InChI=1S/C14H23NO3/c1-4-9(2)5-14(17)18-11-6-10-7-13(16)12(8-11)15(10)3/h4,10-13,15,17-18,20-21,23-24H,22H2,25H3/t12

InChIKey: SIRHVTNTYJCTPI-SCEAUGIDSA-N

Formula: C14H23NO3

SMILES: CC=C(C)CC(=O)OC1CC2CC(O)C(C1)N2C

Mol. weight [g/mol]: 253.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	1.482		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
rinpol	1910.00		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=R577858&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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