

13«alpha»-Isobutyryloxylupanine

Inchi: InChI=1S/C19H30N2O3/c1-12(2)19(23)24-15-6-7-16-14-8-13(9-20(16)11-15)17-4-3-5-18
InchiKey: HHOXDCWBFLNXCK-WALXCBACSA-N
Formula: C19H30N2O3
SMILES: CC(C)C(=O)OC1CCC2C3CC(CN2C1)C1CCCC(=O)N1C3
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	2.049		Crippen Method
mcvol	264.100	ml/mol	McGowan Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R263846&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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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