

4«beta»-Tigloyloxylupanine

Inchi: InChI=1S/C20H30N2O3/c1-3-13(2)20(24)25-16-9-18-14-8-15(12-22(18)19(23)10-16)17-6
InchiKey: ZXQKTNFASBQCFS-VFMSDNQISA-N
Formula: C20H30N2O3
SMILES: CC=C(C)C(=O)OC1CC(=O)N2CC3CC(CN4CCCCC34)C2C1
Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.360		Crippen Method
mcvol	273.890	ml/mol	McGowan Method
rinpole	2864.00		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=R417573&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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