13-Angeloyloxylupanine

Inchi: InChI=1S/C20H30N2O3/c1-3-13(2)20(24)25-19-15-11-14(16-7-4-5-10-21(16)19)12-22-17

InchiKey: ZCUSRGNNIWPAKJ-CKPNNHBISA-N

Formula: C20H30N2O3

SMILES: CC=C(C)C(=O)OC1C2CC(CN3C(=O)CCCC23)C2CCCCN21

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
logp	2.707		Crippen Method
mcvol	273.890	ml/mol	McGowan Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
rinpol	2732.00		NIST Webbook
rinpol	2770.00		NIST Webbook
rinpol	2732.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R109118&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices