3«beta»-Tigloyloxylupanine

Inchi: InChI=1S/C20H30N2O3/c1-3-13(2)20(24)25-17-7-8-18(23)22-12-14-10-15(19(17)22)11-2
InchiKey: PPUAYTALVXQYQS-WHXRPVAYSA-N
Formula: C20H30N2O3
SMILES: CC=C(C)C(=O)OC1CCC(=O)N2CC3CC(CN4CCCCC34)C12
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
rinpol	2850.00		NIST Webbook
rinpol	2850.00		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=R264052&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.