13a-Tigloyloxylupanine

Other names: 13-Tigloyloxylupanine
Inchi: InChI=1S/C20H30N2O3/c1-3-13(2)20(24)25-16-7-8-21-11-14-9-15(18(21)10-16)12-22-17
InchiKey: UPVPJQNTGLTBPC-DXNYSGJVSA-N
Formula: C20H30N2O3
SMILES: CC=C(C)C(=O)OC1CCN2CC3CC(CN4C(=O)CCCC34)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
rinpol	2753.00		NIST Webbook
rinpol	2753.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383538&Units=SI
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

Legend

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