4«alpha»-Angeloyloxy-3«beta»-hydroxylupanine

Inchi: InChI=1S/C20H28N2O5/c1-3-11(2)20(26)27-15-9-16(23)22-10-12-8-13(17(22)18(15)24)1
InchiKey: BRCTWJKFAXRQBQ-KPQUXXMESA-N
Formula: C20H28N2O5
SMILES: CC=C(C)C(=O)OC1CC(=O)N2CC3CC(C(=O)N4CCCCC34)C2C1O
Mol. weight [g/mol]: 376.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	0.857		Crippen Method
mcvol	281.330	ml/mol	McGowan Method
rinpol	2972.00		NIST Webbook
rinpol	2972.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R205404&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

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