13«alpha»-Benzoyloxylupanine

Inchi: InChI=1S/C22H28N2O3/c25-21-8-4-7-20-16-11-17(13-24(20)21)19-10-9-18(14-23(19)12
InchiKey: YOUPTJYGUDWCEW-YFHPXGLKSA-N
Formula: C22H28N2O3
SMILES: O=C(OC1CCC2C3CC(CN2C1)C1CCCC(=O)N1C3)c1ccccc1
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	2.707		Crippen Method
mcvol	282.610	ml/mol	McGowan Method
rinpol	3100.00		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=R263826&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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