13-Benzoyloxylupanine

Inchi: InChI=1S/C22H28N2O3/c25-20-11-6-10-19-17-13-16(14-24(19)20)18-9-4-5-12-23(18)21

InchiKey: ITLXMVBYRSJRFZ-FAFJLIIVSA-N

Formula: C22H28N2O3

SMILES: O=C(OC1C2CC(CN3C(=O)CCCC23)C2CCCCN21)c1ccccc1

Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	3.055		Crippen Method
mcvol	282.610	ml/mol	McGowan Method
rinpol	3105.00		NIST Webbook
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook
rinpol	3090.00		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=R109123&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