

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)c1cccc1
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/ci9903071>

Legend

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

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