13«alpha»-cis-Cinnamoyloxylupanine

Inchi: InChI=1S/C24H30N2O3/c27-23-8-4-7-22-18-13-19(15-26(22)23)21-11-10-20(16-25(21)1
InchiKey: DHCKHXMBCUZMDX-TWXXOYHDSA-N
Formula: C24H30N2O3
SMILES: O=C(C=Cc1ccccc1)OC1CCC2C3CC(CN2C1)C1CCCC(=O)N1C3
Mol. weight [g/mol]: 394.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.107		Crippen Method
mcvol	306.490	ml/mol	McGowan Method
rinpol	3260.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R263831&Units=SI

Legend

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