13-cis-Cinnamoyloxy-17-oxolupanine

Inchi:	InChI=1S/C24H28N2O4/c27-22-8-4-7-21-18-14-25-13-17(10-11-20(25)19(24(18)29)15-2
InchiKey:	QWTJLOAMIUIARH-XFXZXTDPSA-N
Formula:	C24H28N2O4
SMILES:	O=C(C=Cc1ccccc1)OC1CCC2C3CN4C(=O)CCCC4C(CN2C1)C3=O
Mol. weight [g/mol]:	408.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.286		Crippen Method
mcvol	308.060	ml/mol	McGowan Method
rinpol	3418.00		NIST Webbook
rinpol	3418.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R263920&Units=SI
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

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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