13-Benzoyloxy-17-oxolupanine

Inchi:	InChI=1S/C22H26N2O4/c25-20-8-4-7-19-16-12-23-11-15(28-22(27)14-5-2-1-3-6-14)9-10
InchiKey:	AWQNHENUIAQUCO-UHFFFAOYSA-N
Formula:	C22H26N2O4
SMILES:	O=C(OC1CCC2C3CN4C(=O)CCCC4C(CN2C1)C3=O)c1ccccc1
Mol. weight [g/mol]:	382.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	1.886		Crippen Method
mcvol	284.180	ml/mol	McGowan Method
rinpol	3255.00		NIST Webbook
rinpol	3255.00		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=R263900&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

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