13-Phenylacetyloxy-lupanine

Inchi: InChI=1S/C23H30N2O3/c26-22-7-4-9-25-17-12-18-14-20(8-10-24(18)19(13-17)15-21(22
InchiKey: DOHYJDQOPUVWSM-UHFFFAOYSA-N
Formula: C23H30N2O3
SMILES: O=C(Cc1ccccc1)OC1CCN2C(C1)CC1CC2CC2C(=O)CCCN12
Mol. weight [g/mol]: 382.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	2.573		Crippen Method
mcvol	296.700	ml/mol	McGowan Method
rinpol	3095.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R261266&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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