(E)-Methyl 2-((1'R,6'R,7'S,8a'S)-6'-ethyl-2-oxo-3',5',6',7',8',8a'-

Inchi: InChI=1S/C22H28N2O4/c1-4-14-12-24-10-9-22(17-7-5-6-8-18(17)23-21(22)26)19(24)11-

InchiKey: DAXYUDFNWXHGBE-DTQAZKPQSA-N

Formula: C22H28N2O4

SMILES: CCC1CN2CCC3(C(O)=Nc4ccccc43)C2CC1C(=COC)C(=O)OC

Mol. weight [g/mol]: 384.47

CAS: 76-66-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	3.350		Crippen Method
mcvol	295.040	ml/mol	McGowan Method
rinpol	3009.60		NIST Webbook
rinpol	3009.60		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=C76664&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices