(1'S,3R,4a'S,5a'S,10a'S)-Methyl 1'-methyl-2-oxo-1',4a',5',5a',7',8',10',10a'-octahydr

Inchi: InChI=1S/C21H24N2O4/c1-12-14-10-23-8-7-21(16-5-3-4-6-17(16)22-20(21)25)18(23)9-1
InchiKey: JMIAZDVHNCCPDM-UHFFFAOYSA-N
Formula: C21H24N2O4
SMILES: COC(=O)C1=COC(C)C2CN3CCC4(C(=O)Nc5ccccc54)C3CC12
Mol. weight [g/mol]: 368.43
CAS: 5629-60-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	2.062		Crippen Method
mcvol	270.090	ml/mol	McGowan Method
rinpol	3071.70		NIST Webbook
rinpol	3071.70		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=C5629607&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