Methyl 1,1'-dimethyl-2-oxo-1',4a',5',5a',7',8',10',10a'-octah

Inchi: InChI=1S/C22H26N2O4/c1-13-15-11-24-9-8-22(17-6-4-5-7-18(17)23(2)21(22)26)19(24)1

InchiKey: UTVSHFGLVLURNU-UHFFFAOYSA-N

Formula: C22H26N2O4

SMILES: COC(=O)C1=COC(C)C2CN3CCC4(C(=O)N(C)c5ccccc54)C3CC12

Mol. weight [g/mol]: 382.45

CAS: 13897-71-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	2.087		Crippen Method
mcvol	284.180	ml/mol	McGowan Method
rinpol	2942.00		NIST Webbook
rinpol	2942.00		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=C13897717&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