

(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)=Nc4cccc43)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
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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/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/124-859-1/E-Methyl-2-1R-6R-7S-8aS-6-ethyl-2-oxo-3-5-6-7-8-8a-hexahydro-2H-spiro-in>

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