

7,14-Methano-4H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazepan-17-one

Other names: Lupanine, 17-oxo-

decahydro-17-Oxolupanine

[7S-(7«alpha»,7a«beta»,14«alpha»,14a«alpha»)]-

Inchi: InChI=1S/C15H22N2O2/c18-14-6-3-5-13-11-8-10(9-17(13)14)12-4-1-2-7-16(12)15(11)19

InchiKey: HBYSMHYHSFSCED-UHFFFAOYSA-N

Formula: C15H22N2O2

SMILES: O=C1C2CC(CN3C(=O)CCCC23)C2CCCCN12

Mol. weight [g/mol]: 262.35

CAS: 4697-83-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	1.398		Crippen Method
mcvol	201.870	ml/mol	McGowan Method
rinpol	2373.00		NIST Webbook
rinpol	2364.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2356.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2356.00		NIST Webbook
rinpol	2300.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C4697830&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

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