7,14-Methano-4H,6H-dipyrido[1,2-a:1',2'-e][1,5]dia...
1,2,3,7,9,10,11,13,14,14a-decahydro-, [7S-(7«alpha»,14«alpha»,14a«alpha»)]-

Other names: 11,12-Dehydrolupanine

Inchi: InChI=1S/C15H22N2O/c18-15-6-3-5-14-11-8-12(10-17(14)15)13-4-1-2-7-16(13)9-11/h4,1

Inchikey: [illegible]

Formula: C15H22N2O

SMILES: O=C1CCCC2C3CC(CN12)C1=CCCCN1C3

Mol. weight [g/mol]: 246.35

CAS: 35611-60-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.997		Crippen Method
mcvol	196.000	ml/mol	McGowan Method
rinpol	2190.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35611600&Units=SI

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

Legend

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