7,14-Methano-2H,6H-dipyrido[1,2-a:1',2'-e][1,5]dia... dodecahydro-, [7R-(7«alpha»,7a«alpha»,14«alpha»,14a«alpha»)]-

Other names: 11-Epiaphylline
«alpha»-Isoaphylline
11-oxo-«alpha»-isosparteine
Epiaphylline

Inchi: InChI=1S/C15H24N2O/c18-15-12-9-11(13-5-2-4-8-17(13)15)10-16-7-3-1-6-14(12)16/h11

InchiKey: YQMWQSMYVPLYDI-CRWXNKLISA-N

Formula: C15H24N2O

SMILES: O=C1C2CC(CN3CCCCC23)C2CCCCN12

Mol. weight [g/mol]: 248.36

CAS: 1218-51-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	1.872		Crippen Method
mcvol	200.300	ml/mol	McGowan Method
rinpol	2060.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	2055.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1218515&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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