

# 7,14-Methano-2H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazododecahydro-11-Epiaphylline

Other names:

11-Epiaphylline

«alpha»-Isoaphylline

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

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/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

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

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