

7,14-Methano-4H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazododecahydro-11-Isolupanine

Other names:

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

Isolupanine

11-Isolupanine, (+)-

4-Oxo-2-isosparteine

«alpha»-Isolupanine

(+)-«alpha»-isolupanine

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

InchiKey: JYIJIVLEOETIQ-ZOBORPQBSA-N

Formula: C15H24N2O

SMILES: O=C1CCCC2C3CC(CN12)C1CCCCN1C3

Mol. weight [g/mol]: 248.36

CAS: 486-87-3

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	2107.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook

rinpol	2091.00	NIST Webbook
rinpol	2105.00	NIST Webbook
rinpol	2107.00	NIST Webbook
rinpol	2110.00	NIST Webbook
rinpol	2110.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C486873&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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