

7,14-Methano-4H,6H-dipyrido[1,2-a:1',2'-E][1,5]diazocin-11-one, 7,7a,8,9,10,11,13,14-octahydro-, [7R-(7«alpha»,7a«alpha»,14«alpha»)]-

Other names:	Thermoposine Thermoposine, 1- (7R)-Thermoposine
Inchi:	7,14-Methano-2H,11H-dipyrido[1,2-a:1',2'-e][1,5]diazocin-11-one, 1,3,4,6,7,13,14,14a-octahydro-, (7R,14R,14aS)- InChI=1S/C15H20N2O/c18-15-6-3-5-14-11-8-12(10-17(14)15)13-4-1-2-7-16(13)9-11/h3,5
InchiKey:	FQEQMASDZFXSJI-AGIUHOORSA-N
Formula:	C15H20N2O
SMILES:	O=c1cccc2n1CC1CC2CN2CCCCC12
Mol. weight [g/mol]:	244.33
CAS:	486-90-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.820		Crippen Method
mcvol	191.700	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C486908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices

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