

Lupanine

Other names:	7,14-Methano-4H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazocin-4-one, dodecahydro-, [7S-(7«alpha»,7a«beta»,14«alpha»,14a«alpha»)]- (+)-Lupanine 2-Oxosparteine Lupanin d-Lupanine
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-RQJABVFESA-N
Formula:	C15H24N2O
SMILES:	O=C1CCCC2C3CC(CN12)C1CCCCN1C3
Mol. weight [g/mol]:	248.36
CAS:	550-90-3

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	2159.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2165.00		NIST Webbook
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rinpol	2165.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2165.00		NIST Webbook

rinpol	2160.00	NIST Webbook
rinpol	2165.00	NIST Webbook
rinpol	2170.00	NIST Webbook
rinpol	2160.00	NIST Webbook
rinpol	2159.00	NIST Webbook
rinpol	2160.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.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=C550903&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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