Hydroxylupanine

Other names: 7,14-Methano-4H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazocin-4-one, dodecahydro-9-hydroxy-, [7S-(7«alpha»,7a«beta»,9«beta»,14«alpha»,14a«alpha»)]-
Lupanine, 13«alpha»-hydroxy-
Alkaloid C 2, from Cadia purpurea
Jamaidine
Luparine, hydroxy-
Oxylupanine
13«alpha»-Hydroxylupanine
13-Hydroxylupanin
13-Hydroxylupanine
13-Oxylupanine
d-Hydroxylupanine
Lupanine,13-hydroxy
(+)-13-Hydroxylupanine
7,14-Methano-2H,11H-dipyrido(1,2-a:1',2'-e)(1,5)diazocin-11-one, dodecahydro-2-hydroxy-, (2S-(2«alpha»,7«beta»,7a«beta»,14«beta»,14a«alpha»))-
Hydroxylupanin
Lupanine, hydroxy-
NSC 70827

Inchi: InChI=1S/C15H24N2O2/c18-12-4-5-16-8-10-6-11(14(16)7-12)9-17-13(10)2-1-3-15(17)19

InchiKey: JVYKIBAJVKEZSQ-UHFFFAOYSA-N

Formula: C15H24N2O2

SMILES: O=C1CCCC2C3CC(CN12)C1CC(O)CCN1C3

Mol. weight [g/mol]: 264.36

CAS: 15358-48-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	0.842		Crippen Method
mcvol	206.170	ml/mol	McGowan Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2395.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2408.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2402.00		NIST Webbook
rinpol	2402.00		NIST Webbook

rinpol	2400.00	NIST Webbook
rinpol	2410.00	NIST Webbook
rinpol	2410.00	NIST Webbook
rinpol	2410.00	NIST Webbook
rinpol	2410.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C15358482&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