

Lycorenan-7-one, 5-hydroxy-1-methyl-9,10-[methylenebis(oxy)]-, (5«alpha»)-

Other names:	Hippeastrine Lycorenan-9-one, 6-hydroxy-1-methyl-12,13-[methylenebis(oxy)]-, (6«alpha»)- Trispherine [1,3]Dioxolo[6,7][2]benzopyrano[3,4-g]indole, lycorenan-7-one deriv. (5S,5aS,12bS,12cS)-5-Hydroxy-1-methyl-1,2,3,5,5a,12bs,12c-hexahydro-[1,3]dioxolo[4',5']indole
Inchi:	InChI=1S/C17H17NO5/c1-18-3-2-8-4-11(19)16-14(15(8)18)9-5-12-13(22-7-21-12)6-10(9)
InchiKey:	DGQPIOQRPA G NGB-UHFFFAOYSA-N
Formula:	C17H17NO5
SMILES:	CN1CCC2=CC(O)C3OC(=O)c4cc5c(cc4C3C21)OCO5
Mol. weight [g/mol]:	315.32
CAS:	477-17-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	1.043		Crippen Method
mcvol	213.920	ml/mol	McGowan Method
rinpol	2893.70		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C477178&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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