Harmaline

Other names:	3H-Pyrido[3,4-b]indole, 4,9-dihydro-7-methoxy-1-methyl-
	Harmidine
	3,4-Dihydroharmine
	Armalin
	Dihydroharmine
	Harmine, dihydro-
	1-Methyl-7-methoxy-3,4-dihydro-«beta»-carboline
	3,4-Dihydro-7-methoxy-1-methyl-9H-pyrid[3,4-b]indole
	4,9-Dihydro-7-methoxy-1-methyl-3H-pyrido(3,4-b)indole
	Harmalol methyl ether
	O-Methylharmalol
	NSC 407285
	3,4-Dihydro-7-methoxy-1-methyl-9-pyrid(3,4-b)indole
	7-Methoxy-1-methyl-4,9-dihydro-3H-beta-carboline
Inchi:	InChI=1S/C13H14N2O/c1-8-13-11(5-6-14-8)10-4-3-9(16-2)7-12(10)15-13/h3-4,7,15H,5-6
InchiKey:	RERZNCLIYCABFS-UHFFFAOYSA-N
Formula:	C13H14N2O
SMILES:	COc1ccc2c3c([nH]c2c1)C(C)=NCC3
Mol. weight [g/mol]:	214.26
CAS:	304-21-2

Physical Properties

Property code	Value	Unit	Source
ie	7.38 ± 0.06	eV	NIST Webbook
log10ws	-3.38		Crippen Method
logp	2.060		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
rinpol	2266.00		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

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices