Harmine

Other names:	1-Methyl-7-methoxy-«beta»-carboline
	1-Methyl-7-methoxy-Â«betaÂ»-carboline
	6-Methoxyharman
	7-Methoxy-1-methyl-9H-pyrido(3,4-b)indole
	7-Methoxy-1-methyl-9H-pyrido[3,4-b]indole
	9H-Pyrido[3,4-b]indole, 7-methoxy-1-methyl-
	Banisterin
	Banisterine
	Harmin
	Leucoharmine
	Telepathin
	Telepathine
	Yagein
	Yageine
	Yajeine
Inchi:	InChI=1S/C13H12N2O/c1-8-13-11(5-6-14-8)10-4-3-9(16-2)7-12(10)15-13/h3-7,15H,1-2H
InchiKey:	BXNJHAXVSOCGBA-UHFFFAOYSA-N
Formula:	C13H12N2O
SMILES:	COc1ccc2c(c1)[nH]c1c(C)nccc12
Mol. weight [g/mol]:	212.25
CAS:	442-51-3

Physical Properties

Property code	Value	Unit	Source
ie	7.78 ± 0.06	eV	NIST Webbook
log10ws	-4.48		Aqueous Solubility Prediction Method
logp	2.551		Crippen Method
mcvol	161.480	ml/mol	McGowan Method
rinpol	2291.00		NIST Webbook
tf	541.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	48.80	kJ/mol	536.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C442513&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
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
tf:	Normal melting (fusion) point