9H-Pyrido[3,4-b]indol-7-ol, 1-methyl-

Other names:	Harmol
	«beta»-Carboline, 7-hydroxy-1-methyl-
Inchi:	InChI=1S/C12H10N2O/c1-7-12-10(4-5-13-7)9-3-2-8(15)6-11(9)14-12/h2-6,14-15H,1H3
InchiKey:	SATMZMMKDDTOSQ-UHFFFAOYSA-N
Formula:	C12H10N2O
SMILES:	Cc1nccc2c1[nH]c1cc(O)ccc12
Mol. weight [g/mol]:	198.22
CAS:	487-03-6

Physical Properties

Property code	Value	Unit	Source
ie	7.92 ± 0.06	eV	NIST Webbook
log10ws	-4.09		Crippen Method
logp	2.248		Crippen Method
mcvol	147.390	ml/mol	McGowan Method

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=C487036&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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