

9H-Pyrido(3,4-b)indole, 6-methoxy-1-methyl-

Other names:	6-Methoxy-1-methyl-9H-pyrido(3,4-b)indole «beta»-Carboline, 6-methoxy-1-methyl-
Inchi:	InChI=1S/C13H12N2O/c1-8-13-10(5-6-14-8)11-7-9(16-2)3-4-12(11)15-13/h3-7,15H,1-2H
InchiKey:	XYYVPBBISSKKQB-UHFFFAOYSA-N
Formula:	C13H12N2O
SMILES:	COc1ccc2[nH]c3c(C)nccc3c2c1
Mol. weight [g/mol]:	212.25
CAS:	3589-72-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	2.551		Crippen Method
mcvol	161.480	ml/mol	McGowan Method

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=C3589728&Units=SI

Legend

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

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