beta-CARBOLINE, 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

Physical Properties

Property code	Value	Unit	Source
ie	7.55	eV	Cheméo Relay (1.0)
log10ws	-3.82		Cheméo Relay (1.0)
logp	2.551		Crippen Method
mcvol	161.480	ml/mol	McGowan Method
tf	512.50	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3589728&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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

tf: Normal melting (fusion) point