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

Other names: 6-Methoxy-1-methyl-4,9-dihydro-3H-pyrido(3,4-b)indole
6-Methoxyharmalan
6-Methoxy-1-methyl-3,4-dihydro-«beta»-carboline
6-Methoxyharmalane
3H-Pyrido(3,4-b)indole, 4,9-dihydro-6-methoxy-1-methyl-, monohydrochloride
6-Methoxy-1-methyl-4,9-dihydro-3H-pyrido(3,4-b)indole monohydrochloride

Inchi: InChI=1S/C13H14N2O/c1-8-13-10(5-6-14-8)11-7-9(16-2)3-4-12(11)15-13/h3-4,7,15H,5-6

InchiKey: HMBHRMFLDKKSCT-UHFFFAOYSA-N

Formula: C13H14N2O

SMILES: COc1ccc2[nH]c3c(c2c1)CCN=C3C

Mol. weight [g/mol]: 214.26

CAS: 3589-73-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	2.060		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
rinpol	2242.70		NIST Webbook
rinpol	2242.70		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3589739&Units=SI

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

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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