Melatonin

Other names:	5-Methoxy-N-acetyltryptamine
	Acetamide, N-[2-(5-methoxy-1H-indol-3-yl)ethyl]-
	Acetamide, N-[2-(5-methoxyindol-3-yl)ethyl]-
	Circadin
	Melatonine
	N-(2-(5-methoxyindol-3-yl)ethyl)acetamide
	N-Acetyl-5-methoxytryptamine
	N-[2-(5-Methoxy-1H-indol-3-yl)ethyl]acetamide
	NSC 113928
Inchi:	InChI=1S/C13H16N2O2/c1-9(16)14-6-5-10-8-15-13-4-3-11(17-2)7-12(10)13/h3-4,7-8,15H
InchiKey:	DRLFMBDRBRZALE-UHFFFAOYSA-N
Formula:	C13H16N2O2
SMILES:	COc1ccc2[nH]cc(CCNC(C)=O)c2c1
Mol. weight [g/mol]:	232.28
CAS:	73-31-4

Physical Properties

Property code	Value	Unit	Source
ie	7.03	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
log10ws	-5.09		Aqueous Solubility Prediction Method
logp	1.373		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
rinpol	2451.90		NIST Webbook

Sources

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=C73314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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