

# Indole, 3-(2-acetaminoethyl), 5-methoxy (Melatonin), TMS

Inchi:	InChI=1S/C16H24N2O2Si/c1-12(19)17-9-8-13-11-18(21(3,4)5)16-7-6-14(20-2)10-15(13)
InchiKey:	UKAXNBPGNYCYNS-UHFFFAOYSA-N
Formula:	C16H24N2O2Si
SMILES:	COc1ccc2c(c1)c(CCNC(C)=O)cn2[Si](C)(C)C
Mol. weight [g/mol]:	304.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	3.011		Crippen Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R528960&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R528960&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/48-967-6/Indole-3-2-acetaminoethyl-5-methoxy-Melatonin-TMS.pdf>

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