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)1

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: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R528960&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices