Indole, 3-(2-acetaminoethyl), 6-hydroxy-5-methoxy (Hydroxymelatonin), TMS

Inchi: InChI=1S/C19H32N2O3Si2/c1-14(22)20-10-9-15-13-21(25(3,4)5)17-12-19(24-26(6,7)8)1

InchiKey: ZULHUJOKWCYKBH-UHFFFAOYSA-N

Formula: C19H32N2O3Si2

SMILES: COc1cc2c(CCNC(C)=O)cn([Si](C)(C)C)c2cc1O[Si](C)(C)C

Mol. weight [g/mol]: 392.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	4.225		Crippen Method
rinpol	2520.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R528975&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