

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

InChIKey:

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

Formula:

C19H32N2O3Si2

SMILES:

COc1cc2c(CCN(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

Latest version available from:

<https://www.chemeo.com/cid/56-575-2/Indole-3-2-acetaminoethyl-6-hydroxy-5-methoxy-Hydroxymelatonin-TMS.pdf>

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