

Indole, 3-(2-acetoxyethyl), 5-methoxy (Acetylmethoxytryptophol), TMS

Inchi: InChI=1S/C16H23NO3Si/c1-12(18)20-9-8-13-11-17(21(3,4)5)16-7-6-14(19-2)10-15(13)1
InchiKey: RUBVWKUOSAZRDT-UHFFFAOYSA-N
Formula: C16H23NO3Si
SMILES: COc1ccc2c(c1)c(CCOC(C)=O)cn2[Si](C)(C)C
Mol. weight [g/mol]: 305.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	3.438		Crippen Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R528995&Units=SI>

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/53-443-1/Indole-3-2-acetoxyethyl-5-methoxy-Acetylmethoxytryptophol-TMS.pdf>

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