Indole, 3-(2-pentanoylaminoethyl), 5-methoxy, TMS

Inchi: InChI=1S/C19H30N2O2Si/c1-6-7-8-19(22)20-12-11-15-14-21(24(3,4)5)18-10-9-16(23-2)1

InchiKey: GAUXJMKMZRJQQI-UHFFFAOYSA-N

Formula: C19H30N2O2Si

SMILES: CCCCC(=O)NCCc1cn([Si](C)(C)C)c2ccc(OC)cc12

Mol. weight [g/mol]: 346.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	4.182		Crippen Method
rinpol	2600.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529047&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/30-403-0/Indole-3-2-pentanoylaminoethyl-5-methoxy-TMS.pdf

Generated by Cheméo on 2024-10-12 05:51:33.713553809 +0000 UTC m=+3293156.350523056.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.