

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)
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/ci9903071
Crippen Method:	https://www.cheméo.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

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