

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

Inchi:	InChI=1S/C20H32N2O2Si/c1-6-7-8-9-20(23)21-13-12-16-15-22(25(3,4)5)19-11-10-17(24)
InchiKey:	NBCDJQSTEVJISL-UHFFFAOYSA-N
Formula:	C20H32N2O2Si
SMILES:	CCCCCC(=O)NCCc1cn([Si](C)(C)C)c2ccc(OC)cc12
Mol. weight [g/mol]:	360.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	4.572		Crippen Method
rinpol	2690.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R529027&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/56-199-0/Indole-3-2-hexanoylaminoethyl-5-methoxy-TMS.pdf>

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