

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

Inchi:	InChI=1S/C18H28N2O2Si/c1-6-7-18(21)19-11-10-14-13-20(23(3,4)5)17-9-8-15(22-2)12-
InchiKey:	WAOCLFJJUNYADF-UHFFFAOYSA-N
Formula:	C18H28N2O2Si
SMILES:	CCCC(=O)NCCc1cn([Si](C)(C)C)c2ccc(OC)cc12
Mol. weight [g/mol]:	332.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	3.792		Crippen Method
rinsol	2510.00		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R529007&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
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/25-453-1/Indole-3-2-butanoylaminoethyl-5-methoxy-TMS.pdf>

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