

1H-Indole-3-butanoic acid, 1-(trimethylsilyl)-, trimethylsilyl ester

Other names:	Indole-3-butyric acid, bis-TMS
Inchi:	InChI=1S/C18H29NO2Si2/c1-22(2,3)19-14-15(16-11-7-8-12-17(16)19)10-9-13-18(20)21-
InchiKey:	IDHDOSYAEAFHDX-UHFFFAOYSA-N
Formula:	C18H29NO2Si2
SMILES:	C[Si](C)(C)OC(=O)CCc1cn([Si](C)(C)C)c2ccccc12
Mol. weight [g/mol]:	347.60
CAS:	55429-34-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	5.025		Crippen Method
rinpola	2205.00		NIST Webbook
rinpola	2205.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55429340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

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