

trimethylsilyl 1-trimethylsilyl-5-trimethylsiloxy-3-(2-trimethylsilyl

Other names:	TMS 1-TMS-5-TMSoxy-3-(2-TMSamino)indolepropionate 5-OH-Try, TMS
Inchi:	InChI=1S/C23H44N2O3Si4/c1-29(2,3)24-21(23(26)28-32(10,11)12)15-18-17-25(30(4,5)6
InchiKey:	OPTSZAFVDMCAQY-UHFFFAOYSA-N
Formula:	C23H44N2O3Si4
SMILES:	<chem>C[Si](C)(C)NC(Cc1cn([Si](C)(C)C)c2ccc(O[Si](C)(C)C)cc12)C(=O)O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	508.95
CAS:	69937-47-9

Physical Properties

Property code	Value	Unit	Source
log10ws	1.38		Crippen Method
logp	6.252		Crippen Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		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=C69937479&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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