

Normetadrenaline, tri-TMS

Other names:	Normetanephine tri-TMS Normetanephine, N,O,O-tris-TMS Silanamine, N-[2-[3-methoxy-4-[(trimethylsilyl)oxy]phenyl]-2-[(trimethylsilyl)oxy]ethyl]-1,1,1-trimethyl- Normetanephine, TMS Normetanephine, 3tms derivative
Inchi:	InChI=1S/C18H37NO3Si3/c1-20-17-13-15(11-12-16(17)21-24(5,6)7)18(22-25(8,9)10)14-
InchiKey:	PUHXMHRNROQNGZ-UHFFFAOYSA-N
Formula:	C18H37NO3Si3
SMILES:	COc1cc(C(CN[Si](C)(C)C)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]:	399.75
CAS:	68595-62-0

Physical Properties

Property code	Value	Unit	Source
log10ws	1.25		Crippen Method
logp	5.226		Crippen Method
rinpol	1905.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1905.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68595620&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/49-672-2/Normetadrenaline-tri-TMS.pdf>

Generated by Cheméo on 2024-04-17 23:14:40.150405188 +0000 UTC m=+15684929.070982500.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.