

N-Trifluoroacetyl-O,O'-bis(trimethylsilyl)metaneph

Other names:	Metanephrine, N-TFA-O-TMS
Inchi:	InChI=1S/C18H30F3NO4Si2/c1-22(17(23)18(19,20)21)12-16(26-28(6,7)8)13-9-10-14(15)
InchiKey:	GINZNHCPBCSDMI-UHFFFAOYSA-N
Formula:	C18H30F3NO4Si2
SMILES:	COc1cc(C(CN(C)C(=O)C(F)(F)F)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]:	437.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.52		Crippen Method
logp	4.822		Crippen Method
rinpol	1941.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U72259&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/60-553-1/N-Trifluoroacetyl-O-O-bis-trimethylsilyl-metanephrine.pdf>

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