

Synephrine, N-TFA-O-TMS

Other names:	Hydroxyethafedrine N-TFA-bis-O-TMS
Inchi:	InChI=1S/C17H28F3NO3Si2/c1-21(16(22)17(18,19)20)12-15(24-26(5,6)7)13-8-10-14(11
InchiKey:	IIFYFPXALYIATB-UHFFFAOYSA-N
Formula:	C17H28F3NO3Si2
SMILES:	CN(CC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)cc1)C(=O)C(F)(F)F
Mol. weight [g/mol]:	407.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.40		Crippen Method
logp	4.814		Crippen Method
rinsol	1840.00		NIST Webbook
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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=R83229&Units=SI

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.cheméo.com/cid/41-992-5/Synephrine-N-TFA-O-TMS.pdf>

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