

Adrenaline tetrakis(trimethylsilyl)

Other names:	Epinephrine, tetrakis-TMS Epinephrine, TMS Adrenaline, 4tms derivative
Inchi:	InChI=1S/C21H45NO3Si4/c1-22(26(2,3)4)17-21(25-29(11,12)13)18-14-15-19(23-27(5,6)
InchiKey:	GAEOAXOOVYAKOZ-UHFFFAOYSA-N
Formula:	C21H45NO3Si4
SMILES:	CN(CC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1)[Si](C)(C)C
Mol. weight [g/mol]:	471.93
CAS:	54947-77-2

Physical Properties

Property code	Value	Unit	Source
log10ws	2.56		Crippen Method
logp	6.773		Crippen Method
rinpol	2010.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	2010.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54947772&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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