

1-Methyladenosine, tris(trimethylsilyl) ether

Other names:	9-((2R,3R,4R,5R)-3,4-Bis(trimethylsilyloxy)-5-[(trimethylsilyloxy)methyl]-tetrahydrofuran-2-yl)-9-[(2R,3R,4R,5R)-3,4-Bis(trimethylsilyloxy)-5-[(trimethylsilyloxy)methyl]-tetrahydrofuran-2-yl]adenine
Inchi:	InChI=1S/C20H39N5O4Si3/c1-24-12-23-19-15(18(24)21)22-13-25(19)20-17(29-32(8,9)1
InchiKey:	JYJSRESQDQPCSC-UHFFFAOYSA-N
Formula:	C20H39N5O4Si3
SMILES:	Cn1cnc2c(ncn2C2OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(C)C)c1=N
Mol. weight [g/mol]:	497.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.56		Crippen Method
logp	3.438		Crippen Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/96-515-4/1-Methyladenosine-tris-trimethylsilyl-ether.pdf>

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