1-Methyladenosine,tris(trimethylsilyl) ether

Other names: 9-((2R,3R,4R,5R)-3,4-Bis(trimethylsilyloxy)-5-[(trimethylsilyloxy)methyl]-tetrahydrofuran-2
9-{(2R,3R,4R,5R)-3,4-Bis(trimethylsilyloxy)-5-[(trimethylsilyloxy)methyl]-tetrahydrofuran-2
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