Adenosine, 5'-S-methyl-5'-thio-N-(trimethylsilyl)-2',3'-bis-O-(tri

Other names: 5'-S-Methyl-5'-thioadenosine, N-trimethylsilyl-, bis(trimethylsilyl) ether
Inchi: InChI=1S/C20H39N5O3SSi3/c1-29-11-14-16(27-31(5,6)7)17(28-32(8,9)10)20(26-14)25-1
InchiKey: BAKWXPKBSGCDPL-UHFFFAOYSA-N
Formula: C20H39N5O3SSi3
SMILES: CSCC1OC(n2cnc3c(N[Si](C)(C)C)ncnc32)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 513.88
CAS: 54623-28-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.15		Crippen Method
logp	4.774		Crippen Method
rinpol	2788.00		NIST Webbook
rinpol	2821.00		NIST Webbook
rinpol	2821.00		NIST Webbook
rinpol	2788.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54623288&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