5'-S-Methyl-5'-thioadenosine, bis(trimethylsilyl) deriv.

Inchi: InChI=1S/C17H31N5O3SSi2/c1-26-8-11-13(24-27(2,3)4)14(25-28(5,6)7)17(23-11)22-10-

InchiKey: BJFTXDTWJLXWJZ-UHFFFAOYSA-N

Formula: C17H31N5O3SSi2

SMILES: CSCC1OC(n2cnc3c(N)ncnc32)C(O[Si](C)(C)C)C1O[Si](C)(C)C

Mol. weight [g/mol]: 441.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.59		Crippen Method
logp	3.109		Crippen Method
rinpol	2743.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375728&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices