2'-Deoxyadenosine, 3',5'-bis(O-TMSi)

Other names: 2'-Deoxyadenosine, 3',5'-bis-O-TMS
Inchi: InChI=1S/C16H29N5O3Si2/c1-25(2,3)22-8-12-11(24-26(4,5)6)7-13(23-12)21-10-20-14-1
InchiKey: JJEWTFIJBUOVPH-LAGVYOHYSA-N
Formula: C16H29N5O3Si2
SMILES: C[Si](C)(C)OCC1OC(n2cnc3c(N)ncnc32)CC1O[Si](C)(C)C
Mol. weight [g/mol]: 395.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.18		Crippen Method
logp	2.768		Crippen Method
rinpol	2496.00		NIST Webbook
rinpol	2496.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R144106&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices