N6-TMS-2'-Deoxyadenosine, 3'-O-TBDMS, 5'-OTMS

Inchi: InChI=1S/C22H43N5O3Si3/c1-22(2,3)33(10,11)30-16-12-18(29-17(16)13-28-32(7,8)9)27
InchiKey: VLFBIPUDWQTHFK-UKKPGEIXSA-N
Formula: C22H43N5O3Si3
SMILES: CC(C)(C)[Si](C)(C)OC1CC(n2cnc3c(N[Si](C)(C)C)ncnc32)OC1CO[Si](C)(C)C
Mol. weight [g/mol]: 509.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.70		Crippen Method
logp	5.602		Crippen Method
rinpol	2841.00		NIST Webbook
rinpol	2841.00		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=R246950&Units=SI

Legend

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