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

Other names: 2'-Deoxyadenosine, 3',5'-bis-O-cyclotetramethylene-tertbutylsilyl
Inchi: InChI=1S/C26H45N5O3Si2/c1-25(2,3)35(11-7-8-12-35)32-16-20-19(34-36(26(4,5)6)13-9
InchiKey: SSDYEXYOUNXMRF-MCOCGALXSA-N
Formula: C26H45N5O3Si2
SMILES: CC(C)(C)[Si]1(OCC2OC(n3cnc4c(N)ncnc43)CC2O[Si]2(C(C)(C)C)CCCC2)CCCC1
Mol. weight [g/mol]: 531.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	6.177		Crippen Method
rinpol	3594.00		NIST Webbook
rinpol	3594.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R144111&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