2'-Deoxyadenosine, 3',5'-bis-O-cyclotetramethylene-isopropylsilyl

Other names: 2'-Deoxyadenosine, 3',5'-bis(O-TMIPSi)
Inchi: InChI=1S/C24H41N5O3Si2/c1-17(2)33(9-5-6-10-33)30-14-20-19(32-34(18(3)4)11-7-8-12
InchiKey: TXMCBTGUKLCLLK-MCOCGALXSA-N
Formula: C24H41N5O3Si2
SMILES: CC(C)[Si]1(OCC2OC(n3cnc4c(N)ncnc43)CC2O[Si]2(C(C)C)CCCC2)CCCC1
Mol. weight [g/mol]: 503.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	5.396		Crippen Method
rinpol	3520.00		NIST Webbook
rinpol	3520.00		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=R144097&Units=SI

Legend

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