N6-(cyclotetramethylene-tertbutylsilyl)-Adenosine-2,3',5'-tris-O-TBDMS

Inchi: InChI=1S/C36H71N5O4Si4/c1-33(2,3)46(13,14)42-23-26-28(44-47(15,16)34(4,5)6)29(45

InchiKey: GMYGUWPIBWIFTB-DLAWUUKPSA-N

Formula: C36H71N5O4Si4

SMILES: CC(C)(C)[Si]1(Nc2ncnc3c2ncn3C2OC(CO[Si](C)(C)C(C)(C)C)C(O[Si](C)(C)C(C)(C)C)C2

Mol. weight [g/mol]: 750.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Crippen Method
logp	10.478		Crippen Method
rinpol	3811.00		NIST Webbook
rinpol	3811.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R246876&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices