2'-Deoxyadenosine, 3',5'-bis-O-TBDMS

Other names: 2'-Deoxyadenosine, 3',5'-bis(O-TBDMSi)
Inchi: InChI=1S/C22H41N5O3Si2/c1-21(2,3)31(7,8)28-12-16-15(30-32(9,10)22(4,5)6)11-17(29-
InchiKey: JEDIATUHRBNRLS-RTKIROINSA-N
Formula: C22H41N5O3Si2
SMILES: CC(C)(C)[Si](C)(C)OCC1OC(n2cnc3c(N)ncnc32)CC1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 479.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	5.108		Crippen Method
rinpol	2985.00		NIST Webbook
rinpol	2954.00		NIST Webbook
rinpol	2985.00		NIST Webbook
rinpol	2954.00		NIST Webbook
rinpol	2954.00		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=R144082&Units=SI

Legend

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