2'-Deoxyadenosine, 3',5',N6-tris(O-TBDMSi)

Other names: N6-TBDMS-2'-Deoxyadenosine, 3',5'-bis-O-TBDMS
Inchi: InChI=1S/C28H55N5O3Si3/c1-26(2,3)37(10,11)32-24-23-25(30-18-29-24)33(19-31-23)2
InchiKey: RTUGFHFFYHJWKH-UGGDCYSXSA-N
Formula: C28H55N5O3Si3
SMILES: CC(C)(C)[Si](C)(C)Nc1ncnc2c1ncn2C1CC(O[Si](C)(C)C(C)(C)C)C(CO[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 594.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	7.943		Crippen Method
rinpol	3205.00		NIST Webbook
rinpol	3278.00		NIST Webbook
rinpol	3205.00		NIST Webbook
rinpol	3278.00		NIST Webbook
rinpol	3205.00		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=R144126&Units=SI

Legend

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