Adenosine, 2',3',5'-tris(O-TBDMSi)

Other names: Adenosine, 2',3',5'-tris-O-TBDMS
Inchi: InChI=1S/C28H55N5O4Si3/c1-26(2,3)38(10,11)34-16-19-21(36-39(12,13)27(4,5)6)22(37
InchiKey: YZHKRXBIMOGRMG-ODZZBHCRSA-N
Formula: C28H55N5O4Si3
SMILES: CC(C)(C)[Si](C)(C)OCC1OC(n2cnc3c(N)ncnc32)C(O[Si](C)(C)C(C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 610.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.45		Crippen Method
logp	7.108		Crippen Method
rinpol	3237.00		NIST Webbook
rinpol	3273.00		NIST Webbook
rinpol	3203.00		NIST Webbook
rinpol	3237.00		NIST Webbook
rinpol	3203.00		NIST Webbook
rinpol	3203.00		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=R144428&Units=SI

Legend

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

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