N6-acetyl-2'-Deoxyadenosine, 3'-O-TBDMS, 5'-O-acetyl

Inchi: InChI=1S/C20H31N5O5Si/c1-12(26)24-18-17-19(22-10-21-18)25(11-23-17)16-8-14(15(2

InchiKey: RLDMIDFFGGFMDX-ANGDWKNPSA-N

Formula: C20H31N5O5Si

SMILES: CC(=O)Nc1ncnc2c1ncn2C1CC(O[Si](C)(C)C(C)(C)C)C(COC(C)=O)O1

Mol. weight [g/mol]: 449.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	3.026		Crippen Method
rinpol	3079.00		NIST Webbook
rinpol	3079.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R246836&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices