

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(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
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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/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/49-681-2/N6-acetyl-2-Deoxyadenosine-3-O-TBDMS-5-O-acetyl.pdf>

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