

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

Inchi: InChI=1S/C21H37N5O4Si2/c1-14(27)29-15-10-17(30-16(15)11-28-32(8,9)21(2,3)4)26-13
InchiKey: KWYHXSHFWPIORZ-YJEKIOLLSA-N
Formula: C21H37N5O4Si2
SMILES: CC(=O)OC1CC(n2cnc3c(N[Si](C)(C)C)ncnc32)OC1CO[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 479.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	4.314		Crippen Method
rinpol	3058.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R246945&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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<https://www.cheméo.com/cid/29-695-9/N6-TMS-2-Deoxyadenosine-3-O-acetyl-5-O-TBDMS.pdf>

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