

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

Inchi: InChI=1S/C20H25F6N5O5Si/c1-18(2,3)37(4,5)36-10-6-12(35-11(10)7-34-17(33)20(24,25)
InchiKey: PFBAEXNLUWINEL-PQDIPPBSSA-N
Formula: C20H25F6N5O5Si
SMILES: CC(C)(C)[Si](C)(C)OC1CC(n2cnc3c(NC(=O)C(F)(F)F)ncnc32)OC1COC(=O)C(F)(F)F
Mol. weight [g/mol]: 557.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	4.111		Crippen Method
rinpol	2666.00		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=R246905&Units=SI>

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/14-103-1/N6-TFA-2-Deoxyadenosine-3-O-TBDMS-5-O-TFA.pdf>

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