

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

Inchi:	InChI=1S/C20H25F6N5O5Si/c1-18(2,3)37(4,5)34-7-11-10(36-17(33)20(24,25)26)6-12(35)
InchiKey:	FMVUMWRLGAXMTM-PQDIPPBSSA-N
Formula:	C20H25F6N5O5Si
SMILES:	CC(C)(C)[Si](C)(C)OCC1OC(n2cnc3c(NC(=O)C(F)(F)F)ncnc32)CC1OC(=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	2574.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R246910&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/55-651-8/N6-TFA-2-Deoxyadenosine-3-O-TFA-5-O-TBDMS.pdf>

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