Thymidine, 3'-O-TBDMS, 5'-O-TFA

Inchi:	InChI=1S/C18H27F3N2O6Si/c1-10-8-23(16(26)22-14(10)24)13-7-11(29-30(5,6)17(2,3)4)
InchiKey:	KSTXBZGMBOPNIW-VFRRUGBOSA-N
Formula:	C18H27F3N2O6Si
SMILES:	Cc1cn(C2CC(O[Si](C)(C)C(C)(C)C)C(COC(=O)C(F)(F)F)O2)c(=O)[nH]c1=O
Mol. weight [g/mol]:	452.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.20		Crippen Method
logp	2.147		Crippen Method
rinpol	2437.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R247171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/54-935-4/Thymidine-3-O-TBDMS-5-O-TFA.pdf