thymidine, TMS

Inchi:	InChI=1S/C19H38N2O5Si3/c1-14-12-21(19(22)20-18(14)26-29(8,9)10)17-11-15(25-28(5
InchiKey:	PHZFSBAQGMXQIE-UHFFFAOYSA-N
Formula:	C19H38N2O5Si3
SMILES:	Cc1cn(C2CC(O[Si](C)(C)C)C(CO[Si](C)(C)C)O2)c(=O)nc1O[Si](C)(C)C
Mol. weight [g/mol]:	458.77

Physical Properties

Property code	Value	Unit	Source
log10ws	1.89		Crippen Method
logp	4.125		Crippen Method
rinpol	2400.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R207217&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/21-721-7/thymidine-TMS.pdf

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