

Thymine riboside, TMS

Inchi:	InChI=1S/C22H46N2O6Si4/c1-16-14-24(22(25)23-20(16)30-34(11,12)13)21-19(29-33(8,
InchiKey:	MPCOCYVHJKERIX-OCQFDOBUSAN
Formula:	C22H46N2O6Si4
SMILES:	Cc1cn(C2OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(C)C)c(=O)nc1O[Si](C)(C)C
Mol. weight [g/mol]:	546.95

Physical Properties

Property code	Value	Unit	Source
log10ws	3.38		Crippen Method
logp	4.955		Crippen Method
rinpol	2485.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R95402&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/44-585-4/Thymine-riboside-TMS.pdf>

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