

Thymine deoxyriboside, 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-RTKIROINSA-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	2390.00		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=R95395&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/68-394-0/Thymine-deoxyriboside-TMS.pdf>

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