5,6-Dihydrothymine, TMS

Inchi: InChI=1S/C11H24N2O2Si2/c1-9-8-12-11(15-17(5,6)7)13-10(9)14-16(2,3)4/h9H,8H2,1-7H
InchiKey: KDNQBEAAQBPQFH-UHFFFAOYSA-N
Formula: C11H24N2O2Si2
SMILES: CC1CN=C(O[Si](C)(C)C)N=C1O[Si](C)(C)C
Mol. weight [g/mol]: 272.49

Physical Properties

Property code	Value	Unit	Source
log10ws	1.83		Crippen Method
logp	3.094		Crippen Method
rinpol	1395.90		NIST Webbook
rinpol	1478.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R93757&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices