Pyrimidine, 4,6-dihydroxy-5-nitro, TMS

Inchi: InChI=1S/C10H19N3O4Si2/c1-18(2,3)16-9-8(13(14)15)10(12-7-11-9)17-19(4,5)6/h7H,1-6

InchiKey: WNLPITMGOWUKRO-UHFFFAOYSA-N

Formula: C10H19N3O4Si2

SMILES: C[Si](C)(C)Oc1ncnc(O[Si](C)(C)C)c1[N+](=O)[O-]

Mol. weight [g/mol]: 301.45

Physical Properties

Property code	Value	Unit	Source
log10ws	0.33		Crippen Method
logp	2.812		Crippen Method
rinpol	1565.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R386919&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