

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,1-4H2
InchiKey: WNLPTMGOWUKRO-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/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/11-552-6/Pyrimidine-4-6-dihydroxy-5-nitro-TMS.pdf>

Generated by Cheméo on 2024-04-20 06:00:57.01735144 +0000 UTC m=+15882105.937928760.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.