Pyrimidine, 6-amino-4-hydroxy-5-nitro, TMS

Inchi: InChI=1S/C10H20N4O3Si2/c1-18(2,3)13-9-8(14(15)16)10(12-7-11-9)17-19(4,5)6/h7H,1-
InchiKey: RUROJAYIKQAEAI-UHFFFAOYSA-N
Formula: C10H20N4O3Si2
SMILES: C[Si](C)(C)Nc1ncnc(O[Si](C)(C)C)c1[N+](=O)[O-]
Mol. weight [g/mol]: 300.46

Physical Properties

Property code	Value	Unit	Source
log10ws	0.44		Crippen Method
logp	2.845		Crippen Method
rinpol	1697.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R387076&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