Pyrimidine, 5,6-diamino-4-mercapto, TMS

Inchi: InChI=1S/C13H30N4SSi3/c1-19(2,3)16-11-12(17-20(4,5)6)14-10-15-13(11)18-21(7,8)9/h
InchiKey: RMLCMNMZXYPOBU-UHFFFAOYSA-N
Formula: C13H30N4SSi3
SMILES: C[Si](C)(C)Nc1ncnc(S[Si](C)(C)C)c1N[Si](C)(C)C
Mol. weight [g/mol]: 358.73

Physical Properties

Property code	Value	Unit	Source
log10ws	1.57		Crippen Method
logp	4.897		Crippen Method
rinpol	1891.00		NIST Webbook
rinpol	1891.00		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=R387016&Units=SI

Legend

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