Pyrimidine, 6-amino-4-hydroxy-2-mercapto, TMS

Inchi: InChI=1S/C13H29N3OSSi3/c1-19(2,3)16-11-10-12(17-20(4,5)6)15-13(14-11)18-21(7,8)9

InchiKey: HEGCJTSQBKQETA-UHFFFAOYSA-N

Formula: C13H29N3OSSi3

SMILES: C[Si](C)(C)Nc1cc(O[Si](C)(C)C)nc(S[Si](C)(C)C)n1

Mol. weight [g/mol]: 359.71

Physical Properties

Property code	Value	Unit	Source
log10ws	1.46		Crippen Method
logp	4.864		Crippen Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		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=R387041&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices