Pyrimidine, 6-amino-5-hydroxyacetamino-4-mercapto, TMS

InChI: InChI=1S/C15H32N4O2SSi3/c1-23(2,3)19-14-13(18-12(20)10-21-24(4,5)6)15(17-11-16-1

InchiKey: ZIKGEUBKBUYZPS-UHFFFAOYSA-N

Formula: C15H32N4O2SSi3

SMILES: C[Si](C)(C)Nc1ncnc(S[Si](C)(C)C)c1NC(=O)CO[Si](C)(C)C

Mol. weight [g/mol]: 416.76

Physical Properties

Property code	Value	Unit	Source
log10ws	1.87		Crippen Method
logp	4.440		Crippen Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		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=R387096&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices