

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

**TMS**

**InchiKey:**

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

ZIKGEUBKBUIZPS-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
rmpol	2065.00		NIST Webbook
rmpol	2065.00		NIST Webbook

## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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

**rmpol:** Non-polar retention indices

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<https://www.chemeo.com/cid/50-437-1/Pyrimidine-6-amino-5-hydroxyacetamino-4-mercapto-TMS.pdf>

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