

# Pyrimidin-5-carboxylic acid, 4-hydroxy-2-mercapto, TMS

**Inchi:** InChI=1S/C14H28N2O3SSi3/c1-21(2,3)18-12-11(13(17)19-22(4,5)6)10-15-14(16-12)20-2  
**InchiKey:** PXQFFNCLFYAMJQ-UHFFFAOYSA-N  
**Formula:** C14H28N2O3SSi3  
**SMILES:** C[Si](C)(C)OC(=O)c1cnc(S[Si](C)(C)C)nc1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 388.70

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.23		Crippen Method
logp	4.609		Crippen Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		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=R386697&Units=SI>

## Legend

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

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