

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

<b>Inchi:</b>	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
<b>InchiKey:</b>	HEGCJTSQBKQETA-UHFFFAOYSA-N
<b>Formula:</b>	C13H29N3OSSi3
<b>SMILES:</b>	C[Si](C)(C)Nc1cc(O[Si](C)(C)C)nc(S[Si](C)(C)C)n1
<b>Mol. weight [g/mol]:</b>	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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R387041&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R387041&amp;Units=SI</a>

## Legend

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

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