

# Purine, 6-hydroxy-8-carboxymethylthio, TMS

**Inchi:** InChI=1S/C13H22N4O3SSi2/c1-22(2,3)19-9(18)7-21-13-16-10-11(17-13)14-8-15-12(10)  
**InchiKey:** AHDJCTUBPWIMNS-UHFFFAOYSA-N  
**Formula:** C13H22N4O3SSi2  
**SMILES:** C[Si](C)(C)OC(=O)CSc1nc2ncnc(O[Si](C)(C)C)c2[nH]1  
**Mol. weight [g/mol]:** 370.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.13		Crippen Method
logp	2.555		Crippen Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		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=R386617&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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<https://www.chemeo.com/cid/121-347-2/Purine-6-hydroxy-8-carboxymethylthio-TMS.pdf>

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