

# 6-Thiohypoxanthine, TMS

**Inchi:** InChI=1S/C8H10N4OSSi/c1-15(2,3)13-7-5-6(9-4-10-7)12-8(14)11-5/h4H,1-3H3  
**InchiKey:** FJCJGQXYKDTVJZ-UHFFFAOYSA-N  
**Formula:** C8H10N4OSSi  
**SMILES:** C[Si](C)(C)Oc1ncnc2c1=NC(=S)N=2  
**Mol. weight [g/mol]:** 238.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.43		Crippen Method
logp	0.228		Crippen Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		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=R93985&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/55-857-0/6-Thiohypoxanthine-TMS.pdf>

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