

# 7-methylxanthine, TMS

**Inchi:** InChI=1S/C12H22N4O2Si2/c1-16-8-13-9-10(16)14-12(18-20(5,6)7)15-11(9)17-19(2,3)4/H  
**InchiKey:** BVZKIXHBIQUTNP-UHFFFAOYSA-N  
**Formula:** C12H22N4O2Si2  
**SMILES:** Cn1cnc2c(O[Si](C)(C)C)nc(O[Si](C)(C)C)nc21  
**Mol. weight [g/mol]:** 310.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	2.791		Crippen Method
rinpol	2015.00		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	2019.00		NIST Webbook

## Sources

**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=R94012&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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