

# 9H-Purine, 9-(trimethylsilyl)-2,6-bis[(trimethylsilyl)oxy]-

**Other names:** 9-(Trimethylsilyl)-2,6-bis[(trimethylsilyl)oxy]-9H-purine

9H-Purine, 2,6-bis(trimethylsiloxy)-9-(trimethylsilyl)-

Xanthine, TMS

Xanthine, 3tms derivative

**Inchi:** InChI=1S/C14H28N4O2Si3/c1-21(2,3)18-10-15-11-12(18)16-14(20-23(7,8)9)17-13(11)19

**InchiKey:** XGJGXMUBMBXZQP-UHFFFAOYSA-N

**Formula:** C14H28N4O2Si3

**SMILES:** C[Si](C)(C)Oc1nc(O[Si](C)(C)C)c2ncn([Si](C)(C)C)c2n1

**Mol. weight [g/mol]:** 368.65

**CAS:** 18551-03-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.07		Crippen Method
logp	3.937		Crippen Method
rinpol	2005.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2015.00		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=C18551036&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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