

# Purine, 6-carboxymethylthio, TMS

**Inchi:** InChI=1S/C10H14N4O2SSi/c1-18(2,3)16-7(15)4-17-10-8-9(12-5-11-8)13-6-14-10/h5-6H,  
**InchiKey:** UKSGYQKVJRSUOI-UHFFFAOYSA-N  
**Formula:** C10H14N4O2SSi  
**SMILES:** C[Si](C)(C)OC(=O)CSc1ncnc2nc[nH]c12  
**Mol. weight [g/mol]:** 282.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	1.341		Crippen Method
rinpol	2360.00		NIST Webbook
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## 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=R386588&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-409-7/Purine-6-carboxymethylthio-TMS.pdf>

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