

# Purine, 8,9-dimethyl-6-mercapto, TMS

**Inchi:** InChI=1S/C10H16N4SSi/c1-7-13-9-8(14(7)2)10(12-6-11-9)15-16(3,4)5/h6H,1-5H3  
**InchiKey:** UKXIOBPLQYRVLX-UHFFFAOYSA-N  
**Formula:** C10H16N4SSi  
**SMILES:** Cc1nc2ncnc(S[Si](C)(C)C)c2n1C  
**Mol. weight [g/mol]:** 252.41

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -3.97   |      | Crippen Method |
| logp          | 2.599   |      | Crippen Method |
| rinpol        | 1950.00 |      | NIST Webbook   |
| rinpol        | 1950.00 |      | 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=R386662&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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