# 1,3,7-Trimethylxanthine, TMS

**Inchi:** InChI=1S/C8H12N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4-6H,1-3H3
**InchiKey:** PKROKIUCEJBAQW-UHFFFAOYSA-N
**Formula:** C8H12N4O2
**SMILES:** CN1C(=O)C2C(N=CN2C)N(C)C1=O
**Mol. weight [g/mol]:** 196.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | 0.42 | | Crippen Method |
| logp | -0.821 | | Crippen Method |
| mcvol | 140.620 | ml/mol | McGowan Method |
| rinpol | 1800.00 | | NIST Webbook |
| rinpol | 1800.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R22061&Units=SI

## Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**rinpol:** Non-polar retention indices

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