

# Xanthine, 1-(5'-hydroxyhexyl)-3,7-dimethyl

**Inchi:** InChI=1S/C13H20N4O3/c1-9(18)6-4-5-7-17-12(19)10-11(14-8-15(10)2)16(3)13(17)20/h8  
**InchiKey:** NSMXQKNUPPXBRG-UHFFFAOYSA-N  
**Formula:** C13H20N4O3  
**SMILES:** CC(O)CCCCn1c(=O)c2c(ncn2C)n(C)c1=O  
**Mol. weight [g/mol]:** 280.32

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.77   |        | Crippen Method |
| logp          | -0.015  |        | Crippen Method |
| mcvol         | 212.640 | ml/mol | McGowan Method |
| rinpole       | 2430.00 |        | NIST Webbook   |
| rinpole       | 2430.00 |        | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=R146093&Units=SI>

## Legend

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

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