# Barbituric acid, 5-(2-propenyl)-5-(2-hydroxypropyl)

**Inchi:** InChI=1S/C10H14N2O4/c1-3-4-10(5-6(2)13)7(14)11-9(16)12-8(10)15/h3,6,13H,1,4-5H2,
**InchiKey:** VNLMRPAWAMPLNZ-UHFFFAOYSA-N
**Formula:** C10H14N2O4
**SMILES:** C=CCC1(CC(C)O)C(=O)NC(=O)NC1=O
**Mol. weight [g/mol]:** 226.23
**CAS:** 42013-22-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -191.49 | kJ/mol | Joback Method |
| hf | -549.73 | kJ/mol | Joback Method |
| hfus | 24.19 | kJ/mol | Joback Method |
| hvap | 79.01 | kJ/mol | Joback Method |
| log10ws | -1.57 | | Crippen Method |
| logp | -0.314 | | Crippen Method |
| mcvol | 167.140 | ml/mol | McGowan Method |
| pc | 3759.17 | kPa | Joback Method |
| rinpol | 1837.00 | | NIST Webbook |
| rinpol | 1837.00 | | NIST Webbook |
| tb | 836.97 | K | Joback Method |
| tc | 1077.73 | K | Joback Method |
| tf | 692.52 | K | Joback Method |
| vc | 0.616 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 524.14 | J/mol×K | 836.97 | Joback Method |
| cpg | 538.60 | J/mol×K | 877.10 | Joback Method |
| cpg | 552.29 | J/mol×K | 917.22 | Joback Method |
| cpg | 565.23 | J/mol×K | 957.35 | Joback Method |
| cpg | 577.43 | J/mol×K | 997.48 | Joback Method |
| cpg | 588.90 | J/mol×K | 1037.60 | Joback Method |
| cpg | 599.66 | J/mol×K | 1077.73 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C42013229&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |