# Butabarbital M (OH, -H2O)

**Inchi:** InChI=1S/C10H14N2O3/c1-4-6(3)10(5-2)7(13)11-9(15)12-8(10)14/h4H,5H2,1-3H3,(H2,1
**InchiKey:** BNEFYUSURPWDHG-GQCTYLIASA-N
**Formula:** C10H14N2O3
**SMILES:** CC=C(C)C1(CC)C(=O)NC(=O)NC1=O
**Mol. weight [g/mol]:** 210.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -68.40 | kJ/mol | Joback Method |
| hf | -410.22 | kJ/mol | Joback Method |
| hfus | 23.80 | kJ/mol | Joback Method |
| hvap | 63.43 | kJ/mol | Joback Method |
| log10ws | -2.20 | | Crippen Method |
| logp | 0.715 | | Crippen Method |
| mcvol | 161.270 | ml/mol | McGowan Method |
| pc | 3395.98 | kPa | Joback Method |
| rinpol | 1905.00 | | NIST Webbook |
| rinpol | 1905.00 | | NIST Webbook |
| tb | 752.59 | K | Joback Method |
| tc | 1020.22 | K | Joback Method |
| tf | 629.42 | K | Joback Method |
| vc | 0.603 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 469.52 | J/mol×K | 752.59 | Joback Method |
| cpg | 487.16 | J/mol×K | 797.19 | Joback Method |
| cpg | 503.91 | J/mol×K | 841.80 | Joback Method |
| cpg | 519.80 | J/mol×K | 886.40 | Joback Method |
| cpg | 534.87 | J/mol×K | 931.01 | Joback Method |
| cpg | 549.14 | J/mol×K | 975.61 | Joback Method |
| cpg | 562.65 | J/mol×K | 1020.22 | 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=R57327&Units=SI |

# Legend

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|---|---|
| **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 |