

# Butobarbital M (oxo)

**Inchi:** InChI=1S/C10H14N2O4/c1-3-6(13)5-10(4-2)7(14)11-9(16)12-8(10)15/h3-5H2,1-2H3,(H2)  
**InchiKey:** RNMSSWRCPMMUDI-UHFFFAOYSA-N  
**Formula:** C10H14N2O4  
**SMILES:** CCC(=O)CC1(CC)C(=O)NC(=O)NC1=O  
**Mol. weight [g/mol]:** 226.23

## Physical Properties

Property code	Value	Unit	Source
gf	-268.99	kJ/mol	Joback Method
hf	-630.23	kJ/mol	Joback Method
hfus	26.50	kJ/mol	Joback Method
hvap	70.13	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	0.118		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpola	1880.00		NIST Webbook
rinpola	1880.00		NIST Webbook
tb	802.42	K	Joback Method
tc	1059.76	K	Joback Method
tf	698.39	K	Joback Method
vc	0.627	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.34	J/mol×K	802.42	Joback Method
cpg	525.62	J/mol×K	845.31	Joback Method
cpg	540.96	J/mol×K	888.20	Joback Method
cpg	555.35	J/mol×K	931.09	Joback Method
cpg	568.80	J/mol×K	973.98	Joback Method
cpg	581.30	J/mol×K	1016.87	Joback Method
cpg	592.85	J/mol×K	1059.76	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R57359&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R57359&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

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

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