

# Brallobarbital M (des-Br, OH)

**Inchi:** InChI=1S/C10H12N2O4/c1-3-4-10(5-6(2)13)7(14)11-9(16)12-8(10)15/h3H,1,4-5H2,2H3,  
**InchiKey:** NUGVFEZFAAGPMS-UHFFFAOYSA-N  
**Formula:** C10H12N2O4  
**SMILES:** C=CCC1(CC(C)=O)C(=O)NC(=O)NC1=O  
**Mol. weight [g/mol]:** 224.21

## Physical Properties

Property code	Value	Unit	Source
gf	-181.15	kJ/mol	Joback Method
hf	-504.80	kJ/mol	Joback Method
hfus	25.22	kJ/mol	Joback Method
hvap	69.47	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	-0.106		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpola	1795.00		NIST Webbook
rinpola	1795.00		NIST Webbook
tb	799.10	K	Joback Method
tc	1061.51	K	Joback Method
tf	696.63	K	Joback Method
vc	0.609	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.30	J/molxK	799.10	Joback Method
cpg	499.00	J/molxK	842.83	Joback Method
cpg	513.78	J/molxK	886.57	Joback Method
cpg	527.67	J/molxK	930.30	Joback Method
cpg	540.68	J/molxK	974.04	Joback Method
cpg	552.80	J/molxK	1017.77	Joback Method
cpg	564.06	J/molxK	1061.51	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=R57288&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R57288&amp;Units=SI</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>hvap:</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>rinpola:</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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