

# Amobarbital M (OH, -H2O)

**Inchi:** InChI=1S/C11H16N2O3/c1-4-11(6-5-7(2)3)8(14)12-10(16)13-9(11)15/h5H,4,6H2,1-3H3,  
**InchiKey:** VDVCBHJNKZNXT-UHFFFAOYSA-N  
**Formula:** C11H16N2O3  
**SMILES:** CCC1(CC=C(C)C)C(=O)NC(=O)NC1=O  
**Mol. weight [g/mol]:** 224.26

## Physical Properties

Property code	Value	Unit	Source
gf	-59.98	kJ/mol	Joback Method
hf	-430.86	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	65.65	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	1.105		Crippen Method
mvol	175.360	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	775.47	K	Joback Method
tc	1036.79	K	Joback Method
tf	640.69	K	Joback Method
vc	0.658	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.28	J/molxK	775.47	Joback Method
cpg	542.41	J/molxK	819.02	Joback Method
cpg	559.62	J/molxK	862.58	Joback Method
cpg	575.93	J/molxK	906.13	Joback Method
cpg	591.38	J/molxK	949.68	Joback Method
cpg	606.01	J/molxK	993.24	Joback Method
cpg	619.86	J/molxK	1036.79	Joback Method

# Sources

<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=R57274&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R57274&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>

# 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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