

# 2(3H)-Naphthalenone,4,4a,5,6,7,8-hexahydro-4a-m

<b>Inchi:</b>	InChI=1S/C11H16O/c1-11-6-3-2-4-9(11)8-10(12)5-7-11/h8H,2-7H2,1H3
<b>InchiKey:</b>	OHERZLWVBJCXOF-UHFFFAOYSA-N
<b>Formula:</b>	C11H16O
<b>SMILES:</b>	CC12CCCCC1=CC(=O)CC2
<b>Mol. weight [g/mol]:</b>	164.24
<b>CAS:</b>	826-56-2

## Physical Properties

Property code	Value	Unit	Source
gf	14.80	kJ/mol	Joback Method
hf	-205.22	kJ/mol	Joback Method
hfus	5.09	kJ/mol	Joback Method
hvap	44.95	kJ/mol	Joback Method
ie	9.60 ± 0.20	eV	NIST Webbook
log10ws	-3.11		Crippen Method
logp	2.856		Crippen Method
mcvol	141.400	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	558.51	K	Joback Method
tc	807.11	K	Joback Method
tf	345.17	K	Joback Method
vc	0.525	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.72	J/mol×K	558.51	Joback Method
cpg	373.36	J/mol×K	599.94	Joback Method
cpg	391.65	J/mol×K	641.38	Joback Method
cpg	408.77	J/mol×K	682.81	Joback Method
cpg	424.89	J/mol×K	724.24	Joback Method
cpg	440.18	J/mol×K	765.68	Joback Method
cpg	454.79	J/mol×K	807.11	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=C826562&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C826562&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>ie:</b>	Ionization energy
<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>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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