

# 2(1H)-Naphthalenone, octahydro-1-methyl-, (1«alpha»,4a«beta»,8a«alpha»)-

Other names:

2(1H)-Naphthalenone, octahydro-1-methyl-, anti-trans-  
1-Methyl-2-decalone  
2(1H)-Naphthalenone, octahydro-1-methyl-, (1«alpha»,4a«beta»,8a.al  
Bicyclo[4.4.0]decan-3-one,2-methyl-  
2(1H)-Naphthalenone, octahydro-1-methyl-

Inchi:	InChI=1S/C11H18O/c1-8-10-5-3-2-4-9(10)6-7-11(8)12/h8-10H,2-7H2,1H3
InchiKey:	OATKSURGQMWHRL-UHFFFAOYSA-N
Formula:	C11H18O
SMILES:	CC1C(=O)CCC2CCCC21
Mol. weight [g/mol]:	166.26
CAS:	21102-88-5

## Physical Properties

Property code	Value	Unit	Source
gf	-15.46	kJ/mol	Joback Method
hf	-307.45	kJ/mol	Joback Method
hfus	12.70	kJ/mol	Joback Method
hvap	44.53	kJ/mol	Joback Method
ie	9.32 ± 0.08	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.792		Crippen Method
mcvol	145.700	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	544.79	K	Joback Method
tc	779.52	K	Joback Method
tf	299.51	K	Joback Method
vc	0.539	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.04	J/mol×K	544.79	Joback Method
cpg	397.51	J/mol×K	583.91	Joback Method
cpg	418.65	J/mol×K	623.03	Joback Method

cpg	438.51	J/mol×K	662.15	Joback Method
cpg	457.09	J/mol×K	701.27	Joback Method
cpg	474.42	J/mol×K	740.39	Joback Method
cpg	490.52	J/mol×K	779.52	Joback Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21102885&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21102885&amp;Units=SI</a>

## Legend

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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