

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)CCC2CCCCC21
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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21102885&Units=SI

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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