

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

Other names:	«delta»(Sup1,9)-2-Octalone 4,4a,5,6,7,8-Hexahydronaphthalen-2(3H)-one «delta»1,9-2-Octalone «delta»(1(2))-Bicyclo[4.4.0]decenone-3 4,4a,5,6,7,8-Hexahydro 2(3H)-naphthalenone
Inchi:	InChI=1S/C10H14O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h7-8H,1-6H2
InchiKey:	FOCKPZOFYCTNIA-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	O=C1C=C2CCCCC2CC1
Mol. weight [g/mol]:	150.22
CAS:	1196-55-0

Physical Properties

Property code	Value	Unit	Source
gf	11.87	kJ/mol	Joback Method
hf	-199.82	kJ/mol	Joback Method
hfus	8.80	kJ/mol	Joback Method
hvap	43.88	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.466		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1299.00		NIST Webbook
rinpol	1299.00		NIST Webbook
tb	535.39	K	Joback Method
tc	778.59	K	Joback Method
tf	310.00	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.57	J/mol×K	535.39	Joback Method
cpg	325.71	J/mol×K	575.92	Joback Method

cpg	343.65	J/mol×K	616.46	Joback Method
cpg	360.42	J/mol×K	656.99	Joback Method
cpg	376.04	J/mol×K	697.53	Joback Method
cpg	390.57	J/mol×K	738.06	Joback Method
cpg	404.02	J/mol×K	778.59	Joback Method

Sources

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=C1196550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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