

2(1H)-Naphthalenone, 3,4-dihydro-

Other names:	«beta»-Tetralone 2-Tetralone 3,4-Dihydro-2(1H)naphthalenone 1,2,3,4-Tetrahydro-2-naphthalenone 1,2,3,4-tetrahydronaphthalen-2-one
Inchi:	InChI=1S/C10H10O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-4H,5-7H2
InchiKey:	KCKZIWSINLBROE-UHFFFAOYSA-N
Formula:	C10H10O
SMILES:	O=C1CCc2ccccc2C1
Mol. weight [g/mol]:	146.19
CAS:	530-93-8

Physical Properties

Property code	Value	Unit	Source
gf	69.87	kJ/mol	Joback Method
hf	-75.39	kJ/mol	Joback Method
hfus	9.78	kJ/mol	Joback Method
hvap	45.43	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.744		Crippen Method
mvol	118.710	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	543.36	K	Joback Method
tc	792.93	K	Joback Method
tf	328.28	K	Joback Method
vc	0.445	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.39	J/mol×K	543.36	Joback Method
cpg	283.94	J/mol×K	584.96	Joback Method

cpg	298.44	J/mol×K	626.55	Joback Method
cpg	311.91	J/mol×K	668.15	Joback Method
cpg	324.40	J/mol×K	709.74	Joback Method
cpg	335.96	J/mol×K	751.34	Joback Method
cpg	346.61	J/mol×K	792.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	404.20	K	1.50	NIST Webbook
tbrp	411.20	K	2.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C530938&Units=SI
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

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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