

1(2H)-Naphthalenone, 3,4-dihydro-5,7-dimethyl-

Other names:	5,7-Dimethyl-1-tetralone
	5,7-Dimethyl-3,4-dihydro-1(2H)-naphthalenone
	3,4-dihydro-5,7-dimethylnaphthalen-1(2H)-one
Inchi:	InChI=1S/C12H14O/c1-8-6-9(2)10-4-3-5-12(13)11(10)7-8/h6-7H,3-5H2,1-2H3
InchiKey:	UYJCNOMEGPDXMV-UHFFFAOYSA-N
Formula:	C12H14O
SMILES:	Cc1cc(C)c2c(c1)C(=O)CCC2
Mol. weight [g/mol]:	174.24
CAS:	13621-25-5

Physical Properties

Property code	Value	Unit	Source
gf	67.45	kJ/mol	Joback Method
hf	-139.61	kJ/mol	Joback Method
hfus	14.18	kJ/mol	Joback Method
hvap	51.21	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.822		Crippen Method
mcvol	146.890	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	599.08	K	Joback Method
tc	840.31	K	Joback Method
tf	375.86	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.80	J/mol×K	599.08	Joback Method
cpg	378.40	J/mol×K	639.28	Joback Method
cpg	393.98	J/mol×K	679.49	Joback Method
cpg	408.56	J/mol×K	719.69	Joback Method
cpg	422.18	J/mol×K	759.90	Joback Method
cpg	434.85	J/mol×K	800.10	Joback Method

cpg

446.60

J/mol×K

840.31

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.20	K	0.03	NIST Webbook

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=C13621255&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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