1(2H)-Naphthalenone, 3,4-dihydro-3,3,6,8-tetramethyl-

Other names: 3,3,6,8-Tetramethyl-1-tetralone
3,3,6,8-Tetramethyl-3,4-dihydro-1(2H)-naphthalenone
3,4-dihydro-3,3,6,8-tetramethylnaphthalen-1(2H)-one
Inchi: InChI=1S/C14H18O/c1-9-5-10(2)13-11(6-9)7-14(3,4)8-12(13)15/h5-6H,7-8H2,1-4H3
InchiKey: SHSYEGQDGZAMNV-UHFFFAOYSA-N
Formula: C14H18O
SMILES: Cc1cc(C)c2c(c1)CC(C)(C)CC2=O
Mol. weight [g/mol]: 202.29
CAS: 5409-55-2

Physical Properties

Property code	Value	Unit	Source
gf	71.09	kJ/mol	Joback Method
hf	-185.99	kJ/mol	Joback Method
hfus	14.14	kJ/mol	Joback Method
hvap	54.20	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.459		Crippen Method
mcvol	175.070	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
tb	640.41	K	Joback Method
tc	881.06	K	Joback Method
tf	418.06	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.43	J/mol×K	640.41	Joback Method
cpg	479.58	J/mol×K	680.52	Joback Method
cpg	496.78	J/mol×K	720.63	Joback Method
cpg	513.18	J/mol×K	760.73	Joback Method
cpg	528.91	J/mol×K	800.84	Joback Method
cpg	544.11	J/mol×K	840.95	Joback Method

cpg	558.92	J/mol×K	881.06	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=C5409552&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
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