1(2H)-Naphthalenone, 3,4-dihydro-5,8-dimethyl-

Other names: 5,8-Dimethyl-3,4-dihydro-1(2H)-naphthalenone
5,8-Dimethyltetralone

Inchi: InChI=1S/C12H14O/c1-8-6-7-9(2)12-10(8)4-3-5-11(12)13/h6-7H,3-5H2,1-2H3

InchiKey: ZSMGKPHICFZGQU-UHFFFAOYSA-N

Formula: C12H14O

SMILES: Cc1ccc(C)c2c1CCCC2=O

Mol. weight [g/mol]: 174.24

CAS: 5037-63-8

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	305.20 ± 2.00	K	NIST Webbook
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

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=C5037638&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume