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

Other names:	3,4-dihydro-6-methoxy-1(2H)naphthalenone
	6-Methoxy-1,2,3,4-tetrahydro-1-naphthalenone
	6-Methoxy-«alpha»-tetralone
	6-methoxy-1,2,3,4-tetrahydronaphthalen-1-one
	6-methoxy-1-tetralone
	6-methoxy-3,4-dihydro-1(2H)-naphthalenone
Inchi:	InChI=1S/C11H12O2/c1-13-9-5-6-10-8(7-9)3-2-4-11(10)12/h5-7H,2-4H2,1H3
InchiKey:	MNALUTYMBUBKNX-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	COc1ccc2c(c1)CCCC2=O
Mol. weight [g/mol]:	176.21
CAS:	1078-19-9

Physical Properties

Property code	Value	Unit	Source
gf	-36.34	kJ/mol	Joback Method
hf	-239.72	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hsub	104.70 ± 0.90	kJ/mol	NIST Webbook
hvap	50.73	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.214		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	593.64	K	Joback Method
tc	835.26	K	Joback Method
tf	374.30	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.90	J/mol×K	593.64	Joback Method
cpg	354.65	J/mol×K	633.91	Joback Method

cpg	369.43	J/mol×K	674.18	Joback Method
cpg	383.26	J/mol×K	714.45	Joback Method
cpg	396.14	J/mol×K	754.72	Joback Method
cpg	408.08	J/mol×K	794.99	Joback Method
cpg	419.09	J/mol×K	835.26	Joback Method
hfust	22.80	kJ/mol	351.30	NIST Webbook
hvapt	104.70	kJ/mol	298.15	Thermochemical study of some methoxytetralones

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	444.20	K	1.50	NIST Webbook

Sources

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=C1078199&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermochemical study of some methoxytetralones: https://www.doi.org/10.1016/j.jct.2008.07.021

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

hfust: Enthalpy of fusion at a given temperature

hsub: Enthalpy of sublimation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

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