

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

Other names:	6-Methoxy-2-tetralone 6-methoxy-1,2,3,4-tetrahydronaphthalen-2-one
Inchi:	InChI=1S/C11H12O2/c1-13-11-5-3-8-6-10(12)4-2-9(8)7-11/h3,5,7H,2,4,6H2,1H3
InchiKey:	RMRKDYNVZWKAFF-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	COc1ccc2c(c1)CCC(=O)C2
Mol. weight [g/mol]:	176.21
CAS:	2472-22-2

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
hvap	50.73	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.753		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/molxK	593.64	Joback Method
cpg	354.65	J/molxK	633.91	Joback Method
cpg	369.43	J/molxK	674.18	Joback Method
cpg	383.26	J/molxK	714.45	Joback Method
cpg	396.14	J/molxK	754.72	Joback Method
cpg	408.08	J/molxK	794.99	Joback Method
cpg	419.09	J/molxK	835.26	Joback Method

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=C2472222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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