

# 7-Methoxy-1-tetralone

<b>Other names:</b>	1(2H)-Naphthalenone, 3,4-dihydro-7-methoxy- 3,4-Dihydro-7-methoxy-1(2H)-naphthalenone 7-methoxy-1,2,3,4-tetrahydronaphthalen-1-one
<b>Inchi:</b>	InChI=1S/C11H12O2/c1-13-9-6-5-8-3-2-4-11(12)10(8)7-9/h5-7H,2-4H2,1H3
<b>InchiKey:</b>	GABLTKRIYDNDIN-UHFFFAOYSA-N
<b>Formula:</b>	C11H12O2
<b>SMILES:</b>	<chem>COc1ccc2c(c1)C(=O)CCC2</chem>
<b>Mol. weight [g/mol]:</b>	176.21
<b>CAS:</b>	6836-19-7

## 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	103.10 ± 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	m <sup>3</sup> /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	23.20	kJ/mol	334.80	NIST Webbook
hvapt	103.10	kJ/mol	298.15	Thermochemical study of some methoxytetralones

## Sources

**Thermochemical study of some methoxytetralones:**  
**Joback Method:**

<https://www.doi.org/10.1016/j.jct.2008.07.021>

[https://en.wikipedia.org/wiki/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=C6836197&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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