

# 1(2H)-Naphthalenone, 5-methoxy

<b>Inchi:</b>	InChI=1S/C11H10O2/c1-13-11-7-3-4-8-9(11)5-2-6-10(8)12/h2-5,7H,6H2,1H3
<b>InchiKey:</b>	OCCGHDQBFJYJQT-UHFFFAOYSA-N
<b>Formula:</b>	C11H10O2
<b>SMILES:</b>	COc1cccc2c1C=CCC2=O
<b>Mol. weight [g/mol]:</b>	174.20

## Physical Properties

Property code	Value	Unit	Source
gf	-6.38	kJ/mol	Joback Method
hf	-181.94	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	51.02	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.295		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
tb	592.80	K	Joback Method
tc	836.85	K	Joback Method
tf	375.06	K	Joback Method
vc	0.504	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.49	J/molxK	592.80	Joback Method
cpg	332.96	J/molxK	633.48	Joback Method
cpg	346.52	J/molxK	674.15	Joback Method
cpg	359.17	J/molxK	714.83	Joback Method
cpg	370.92	J/molxK	755.50	Joback Method
cpg	381.79	J/molxK	796.18	Joback Method
cpg	391.80	J/molxK	836.85	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R71779&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R71779&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# 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>hvap:</b>	Enthalpy of vaporization at standard conditions
<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>rinpola:</b>	Non-polar retention indices
<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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