

# 4a«beta»,7«alpha»,7a«beta»-Nepetalactone

**Inchi:** InChI=1S/C10H14O2/c1-6-3-4-8-7(2)5-12-10(11)9(6)8/h5-6,8-9H,3-4H2,1-2H3/t6-,8-,9-/m  
**InchiKey:** ZDKZHVNKFOXMND-FTLITQJKSA-N  
**Formula:** C10H14O2  
**SMILES:** CC1=COC(=O)C2C(C)CCC12  
**Mol. weight [g/mol]:** 166.22

## Physical Properties

Property code	Value	Unit	Source
gf	-77.57	kJ/mol	Joback Method
hf	-366.34	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	47.60	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.109		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1352.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1398.00		NIST Webbook
tb	548.73	K	Joback Method
tc	780.29	K	Joback Method
tf	331.61	K	Joback Method
vc	0.498	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	339.65	J/mol×K	548.73	Joback Method
cpg	357.85	J/mol×K	587.32	Joback Method
cpg	375.01	J/mol×K	625.92	Joback Method
cpg	391.16	J/mol×K	664.51	Joback Method
cpg	406.31	J/mol×K	703.10	Joback Method
cpg	420.46	J/mol×K	741.70	Joback Method
cpg	433.65	J/mol×K	780.29	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=R285737&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R285737&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>rinpol:</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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