

# (4aS,7S,7aR)-4,7-Dimethyl-5,6,7,7a-tetrahydrocycl

<b>Other names:</b>	(+)-(4aS,7S,7aR)-Nepetalactone (+)-cis,trans-Nepetalactone (4aS,7S,7aR)-nepetalactone 4a«alpha»,7«alpha»,7a«alpha»-Nepetalactone 4a«alpha»,7«beta»,7a«alpha»-Nepetalactone Cyclopenta[c]pyran-1(4aH)-one, 5,6,7,7a-tetrahydro-4,7-dimethyl-, (4aS,7S,7aR)- Cyclopenta[c]pyran-1(4aH)-one, 5,6,7,7a-tetrahydro-4,7-dimethyl-, [4aS-(4a«alpha»,7«alpha»,7a«alpha»)]- Cyclopenta[c]pyran-1(4aH)-one, 5,6,7,7a-tetrahydro-4,7«alpha»-dimethyl-, (+)- Nepetalactone, cis-trans- cis-trans-Nepetalactone
<b>Inchi:</b>	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
<b>InchiKey:</b>	ZDKZHVNKFOXMND-UHFFFAOYSA-N
<b>Formula:</b>	C10H14O2
<b>SMILES:</b>	CC1=COC(=O)C2C(C)CCC12
<b>Mol. weight [g/mol]:</b>	166.22
<b>CAS:</b>	21651-62-7

## 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	1377.00		NIST Webbook
rinpol	1377.00		NIST Webbook
tb	548.73	K	Joback Method
tc	780.29	K	Joback Method
tf	331.61	K	Joback Method
vc	0.498	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
hvapt	69.40	kJ/mol	298.15	Vapor pressure and enthalpy of vaporization of oil of catnip by correlation gas chromatography

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21651627&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21651627&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Vapor pressure and enthalpy of vaporization of oil of catnip by Joback Method:	<a href="https://www.doi.org/10.1016/j.jct.2015.09.005">https://www.doi.org/10.1016/j.jct.2015.09.005</a>
chromatography:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## 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
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

<b>rinp0l:</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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