

# (R)-2-((4aS,8aR)-4a-Methyl-8-methylene-1,4,4a,5,6

<b>Other names:</b>	2-Naphthaleneethanol, 1,4,4a,5,6,7,8,8a-octahydro-«beta»,4a-dimethyl-8-methylene-, 2-Naphthaleneethanol, 1,4,4a,5,6,7,8,8a-octahydro-, 5«beta»,10«alpha»-Eudesma-4(14),7-dien-12-ol, (11R)- [4aS-[2(S*),4A«alpha»,8a«beta»]]- Vetiselinenol
<b>Inchi:</b>	InChI=1S/C15H24O/c1-11-5-4-7-15(3)8-6-13(9-14(11)15)12(2)10-16/h6,12,14,16H,1,4-5
<b>InchiKey:</b>	RQWRGJGCTMAFBS-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	C=C1CCCC2(C)CC=C(C(C)CO)CC12
<b>Mol. weight [g/mol]:</b>	220.35
<b>CAS:</b>	28102-68-3

## Physical Properties

Property code	Value	Unit	Source
gf	77.18	kJ/mol	Joback Method
hf	-243.69	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1723.00		NIST Webbook
rinpol	1723.00		NIST Webbook
tb	668.44	K	Joback Method
tc	875.24	K	Joback Method
tf	377.29	K	Joback Method
vc	0.739	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.07	J/molxK	668.44	Joback Method
cpg	588.18	J/molxK	702.91	Joback Method
cpg	605.40	J/molxK	737.37	Joback Method

cpg	621.84	J/mol×K	771.84	Joback Method
cpg	637.63	J/mol×K	806.31	Joback Method
cpg	652.89	J/mol×K	840.77	Joback Method
cpg	667.74	J/mol×K	875.24	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=C28102683&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C28102683&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>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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