

# (-)-(1S,6S,9R,10R)-9«alpha»-Hydroxyamorpha-4,7

<b>Inchi:</b>	InChI=1S/C15H24O/c1-9(2)13-8-15(16)11(4)12-6-5-10(3)7-14(12)13/h7,11-12,14-16H,5-
<b>InchiKey:</b>	VYRPEQZTLXTRND-JURCDPSOSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC1=CC2C(=C(C)C)CC(O)C(C)C2CC1
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	53.52	kJ/mol	Joback Method
hf	-312.33	kJ/mol	Joback Method
hfus	28.55	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mvol	197.760	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	666.66	K	Joback Method
tc	869.95	K	Joback Method
tf	342.63	K	Joback Method
vc	0.745	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.39	J/molxK	666.66	Joback Method
cpg	597.44	J/molxK	700.54	Joback Method
cpg	615.40	J/molxK	734.42	Joback Method
cpg	632.32	J/molxK	768.31	Joback Method
cpg	648.22	J/molxK	802.19	Joback Method
cpg	663.16	J/molxK	836.07	Joback Method
cpg	677.18	J/molxK	869.95	Joback Method

# Sources

<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>
<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=R515870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R515870&amp;Units=SI</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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