

# 2-hydroxy-1-(4'S-isopropenyl-1-cyclohexen-1-yl)-1

(R,S)

InChI:

InChI=1S/C12H18O2/c1-8(2)10-4-6-11(7-5-10)12(14)9(3)13/h6,9-10,13H,1,4-5,7H2,2-3H

InChIKey:

PZBGMBKRUHYASB-VHSXEESVSA-N

Formula:

C12H18O2

SMILES:

C=C(C)C1CC=C(C(=O)C(C)O)CC1

Mol. weight [g/mol]:

194.27

## Physical Properties

Property code	Value	Unit	Source
gf	-93.95	kJ/mol	Joback Method
hf	-344.83	kJ/mol	Joback Method
hfus	19.08	kJ/mol	Joback Method
hvap	66.14	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.239		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
ripol	2220.00		NIST Webbook
tb	639.82	K	Joback Method
tc	841.74	K	Joback Method
tf	325.69	K	Joback Method
vc	0.627	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.81	J/molxK	639.82	Joback Method
cpg	464.72	J/molxK	673.47	Joback Method
cpg	478.75	J/molxK	707.13	Joback Method
cpg	491.93	J/molxK	740.78	Joback Method
cpg	504.30	J/molxK	774.43	Joback Method
cpg	515.89	J/molxK	808.09	Joback Method
cpg	526.73	J/molxK	841.74	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=R522719&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R522719&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvac:</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</b>	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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