

# 9-Hydroxymegastigm-7-en-3-one

<b>Inchi:</b>	InChI=1S/C13H22O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h5-6,9-10,12,14H,7-8H2,1
<b>InchiKey:</b>	WFSOPDPEWLYCRX-AATRIKPKSA-N
<b>Formula:</b>	C13H22O2
<b>SMILES:</b>	CC(O)C=CC1C(C)CC(=O)CC1(C)C
<b>Mol. weight [g/mol]:</b>	210.31

## Physical Properties

Property code	Value	Unit	Source
gf	-119.51	kJ/mol	Joback Method
hf	-460.76	kJ/mol	Joback Method
hfus	17.38	kJ/mol	Joback Method
hvap	63.69	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.565		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
ripol	2473.00		NIST Webbook
ripol	2473.00		NIST Webbook
tb	671.01	K	Joback Method
tc	879.89	K	Joback Method
tf	368.03	K	Joback Method
vc	0.693	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.16	J/mol×K	671.01	Joback Method
cpg	557.04	J/mol×K	705.82	Joback Method
cpg	574.10	J/mol×K	740.64	Joback Method
cpg	590.41	J/mol×K	775.45	Joback Method
cpg	606.06	J/mol×K	810.26	Joback Method
cpg	621.13	J/mol×K	845.07	Joback Method
cpg	635.72	J/mol×K	879.89	Joback Method

# Sources

<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=R302619&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R302619&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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

Latest version available from:

<https://www.chemeo.com/cid/83-191-8/9-Hydroxymegastigm-7-en-3-one.pdf>

Generated by Cheméo on 2024-04-23 16:49:26.353754772 +0000 UTC m=+16180215.274332093.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.