

# isomustakone

<b>Inchi:</b>	InChI=1S/C14H20O/c1-8(2)9-6-7-14(3)10-4-5-11(15)13(14)12(9)10/h4-5,8-10,12-13H,6-7
<b>InchiKey:</b>	GZLLVGOKTRVUIU-FJTNJNQGSA-N
<b>Formula:</b>	C14H20O
<b>SMILES:</b>	CC(C)C1CCC2(C)C3C=CC(=O)C2C13
<b>Mol. weight [g/mol]:</b>	204.31

## Physical Properties

Property code	Value	Unit	Source
gf	121.17	kJ/mol	Joback Method
hf	-230.69	kJ/mol	Joback Method
hfus	17.37	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.060		Crippen Method
mcvol	172.810	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinqol	1657.00		NIST Webbook
tb	601.65	K	Joback Method
tc	831.96	K	Joback Method
tf	367.24	K	Joback Method
vc	0.665	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.88	J/mol×K	601.65	Joback Method
cpg	512.09	J/mol×K	640.04	Joback Method
cpg	531.96	J/mol×K	678.42	Joback Method
cpg	550.69	J/mol×K	716.81	Joback Method
cpg	568.46	J/mol×K	755.19	Joback Method
cpg	585.45	J/mol×K	793.58	Joback Method
cpg	601.87	J/mol×K	831.96	Joback Method

# Sources

<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>
<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=R334280&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R334280&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>mccvol:</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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