

# 3-Oxo-«alpha»-ionone

<b>Inchi:</b>	InChI=1S/C13H18O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h5-7,12H,8H2,1-4H3/b6-5
<b>InchiKey:</b>	MLYOGKJJENFVJN-AATRIKPKSA-N
<b>Formula:</b>	C13H18O2
<b>SMILES:</b>	CC(=O)C=CC1C(C)=CC(=O)CC1(C)C
<b>Mol. weight [g/mol]:</b>	206.28
<b>CAS:</b>	79734-43-3

## Physical Properties

Property code	Value	Unit	Source
gf	-81.13	kJ/mol	Joback Method
hf	-349.18	kJ/mol	Joback Method
hfus	18.18	kJ/mol	Joback Method
hvap	55.41	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.693		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	641.95	K	Joback Method
tc	872.71	K	Joback Method
tf	389.66	K	Joback Method
vc	0.672	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.42	J/molxK	641.95	Joback Method
cpg	489.28	J/molxK	680.41	Joback Method
cpg	506.22	J/molxK	718.87	Joback Method
cpg	522.33	J/molxK	757.33	Joback Method
cpg	537.74	J/molxK	795.79	Joback Method
cpg	552.56	J/molxK	834.25	Joback Method

## Sources

<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=C79734433&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C79734433&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>
<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>

## 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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