

# 3-Buten-2-one, 4-(2,2-dimethyl-6-methylenecyclohexyl)-

Other names:

«gamma»-Ionone

4-(2,2-dimethyl-6-methylenecyclohexyl)-3-buten-2-one

Inchi: InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h7-8,12H,1,5-6,9H2,2-4H3/b8

InchiKey: SFEOKXHPFMOVRM-BQYQJAHWSA-N

Formula: C13H20O

SMILES: C=C1CCCC(C)(C)C1C=CC(C)=O

Mol. weight [g/mol]: 192.30

CAS: 79-76-5

## Physical Properties

Property code	Value	Unit	Source
gf	74.21	kJ/mol	Joback Method
hf	-173.55	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.514		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
ripol	1340.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1897.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1846.00		NIST Webbook
ripol	1846.00		NIST Webbook
ripol	1882.00		NIST Webbook
tb	569.15	K	Joback Method
tc	785.96	K	Joback Method
tf	321.84	K	Joback Method
vc	0.663	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.42	J/molxK	569.15	Joback Method
cpg	456.28	J/molxK	605.28	Joback Method
cpg	474.02	J/molxK	641.42	Joback Method
cpg	490.76	J/molxK	677.55	Joback Method
cpg	506.62	J/molxK	713.69	Joback Method
cpg	521.73	J/molxK	749.82	Joback Method
cpg	536.20	J/molxK	785.96	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=C79765&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C79765&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>

## 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>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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