

# 2,4-Cyclohexadienone

Inchi:	InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-4H,5H2
InchiKey:	WQPDQJCBHQPNCZ-UHFFFAOYSA-N
Formula:	C6H6O
SMILES:	O=C1C=CC=CC1
Mol. weight [g/mol]:	94.11
CAS:	24599-57-3

## Physical Properties

Property code	Value	Unit	Source
gf	-30.87	kJ/mol	Joback Method
hf	-70.00 ± 10.00	kJ/mol	NIST Webbook
hfus	4.01	kJ/mol	Joback Method
hvap	34.52	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.072		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	427.04	K	Joback Method
tc	659.38	K	Joback Method
tf	238.74	K	Joback Method
vc	0.284	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.24	J/molxK	427.04	Joback Method
cpg	146.34	J/molxK	465.76	Joback Method
cpg	156.91	J/molxK	504.49	Joback Method
cpg	166.94	J/molxK	543.21	Joback Method
cpg	176.43	J/molxK	581.93	Joback Method
cpg	185.38	J/molxK	620.66	Joback Method
cpg	193.78	J/molxK	659.38	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C24599573&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C24599573&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>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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