

# Methyl 1-methylcyclopropyl ketone

<b>Other names:</b>	Ethanone, 1-(1-methylcyclopropyl)- (1-Methylcyclopropyl)(methyl)ketone Ketone, methyl 1-methylcyclopropyl 1-Acetyl-1-methylcyclopropane
<b>Inchi:</b>	InChI=1S/C6H10O/c1-5(7)6(2)3-4-6/h3-4H2,1-2H3
<b>InchiKey:</b>	OQBCJXUAQQMTRW-UHFFFAOYSA-N
<b>Formula:</b>	C6H10O
<b>SMILES:</b>	CC(=O)C1(C)CC1
<b>Mol. weight [g/mol]:</b>	98.14
<b>CAS:</b>	1567-75-5

## Physical Properties

Property code	Value	Unit	Source
gf	-74.02	kJ/mol	Joback Method
hf	-191.71	kJ/mol	Joback Method
hfus	4.73	kJ/mol	Joback Method
hvap	34.46	kJ/mol	Joback Method
ie	9.30	eV	NIST Webbook
log10ws	-1.27		Crippen Method
logp	1.375		Crippen Method
mcvol	86.110	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
tb	399.50 ± 1.50	K	NIST Webbook
tb	399.70	K	NIST Webbook
tc	599.54	K	Joback Method
tf	249.15	K	Joback Method
vc	0.333	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.92	J/mol×K	397.53	Joback Method
cpg	174.06	J/mol×K	431.20	Joback Method
cpg	185.16	J/mol×K	464.87	Joback Method

cpg	195.34	J/mol×K	498.53	Joback Method
cpg	204.68	J/mol×K	532.20	Joback Method
cpg	213.30	J/mol×K	565.87	Joback Method
cpg	221.29	J/mol×K	599.54	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	325.00	K	5.50	NIST Webbook

## 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=C1567755&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1567755&amp;Units=SI</a>
<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>

## 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>ie:</b>	Ionization energy
<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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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