

# Methyloctenone

<b>Inchi:</b>	InChI=1S/C9H16O/c1-8(2)6-4-5-7-9(3)10/h6H,4-5,7H2,1-3H3
<b>InchiKey:</b>	GHJLLLILWMDFDE-UHFFFAOYSA-N
<b>Formula:</b>	C9H16O
<b>SMILES:</b>	CC(=O)CCCC=C(C)C
<b>Mol. weight [g/mol]:</b>	140.22

## Physical Properties

Property code	Value	Unit	Source
gf	-32.35	kJ/mol	Joback Method
hf	-234.24	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	42.41	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.712		Crippen Method
mvol	134.940	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
tb	463.23	K	Joback Method
tc	648.94	K	Joback Method
tf	222.08	K	Joback Method
vc	0.526	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.40	J/mol×K	463.23	Joback Method
cpg	294.83	J/mol×K	494.18	Joback Method
cpg	307.62	J/mol×K	525.13	Joback Method
cpg	319.80	J/mol×K	556.08	Joback Method
cpg	331.40	J/mol×K	587.03	Joback Method
cpg	342.43	J/mol×K	617.99	Joback Method
cpg	352.92	J/mol×K	648.94	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=R520728&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R520728&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>hvp:</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>rinp:</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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