

# Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-

<b>Other names:</b>	2-Pinen-4-one Berbenone Verbenone 4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-one
<b>Inchi:</b>	InChI=1S/C10H14O/c1-6-4-9(11)8-5-7(6)10(8,2)3/h4,7-8H,5H2,1-3H3
<b>InchiKey:</b>	DCSCXTJOXBUFGB-UHFFFAOYSA-N
<b>Formula:</b>	C10H14O
<b>SMILES:</b>	<chem>CC1=CC(=O)C2CC1C2(C)C</chem>
<b>Mol. weight [g/mol]:</b>	150.22
<b>CAS:</b>	80-57-9

## Physical Properties

Property code	Value	Unit	Source
gf	27.26	kJ/mol	Joback Method
hf	-206.78	kJ/mol	Joback Method
hfus	10.94	kJ/mol	Joback Method
hvap	41.59	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
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tb	500.70	K	NIST Webbook
tc	740.08	K	Joback Method
tf	335.98	K	Joback Method
vc	0.491	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.39	J/mol×K	513.48	Joback Method
cpg	324.08	J/mol×K	551.25	Joback Method
cpg	339.67	J/mol×K	589.01	Joback Method
cpg	354.29	J/mol×K	626.78	Joback Method
cpg	368.08	J/mol×K	664.55	Joback Method
cpg	381.17	J/mol×K	702.31	Joback Method
cpg	393.70	J/mol×K	740.08	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=C80579&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C80579&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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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