

# Bicyclo[4.1.0]heptan-2-one, 3,7,7-trimethyl-

<b>Other names:</b>	2-Caranone Caron Carone
<b>Inchi:</b>	InChI=1S/C10H16O/c1-6-4-5-7-8(9(6)11)10(7,2)3/h6-8H,4-5H2,1-3H3
<b>InchiKey:</b>	CNJLMVZFWLNOEP-UHFFFAOYSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	CC1CCC2C(C1=O)C2(C)C
<b>Mol. weight [g/mol]:</b>	152.23
<b>CAS:</b>	497-62-1

## Physical Properties

Property code	Value	Unit	Source
gf	-0.78	kJ/mol	Joback Method
hf	-273.43	kJ/mol	Joback Method
hfus	11.18	kJ/mol	Joback Method
hvap	40.33	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpola	1252.00		NIST Webbook
ripola	1634.00		NIST Webbook
tb	504.67	K	Joback Method
tc	727.60	K	Joback Method
tf	318.46	K	Joback Method
vc	0.504	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.94	J/molxK	504.67	Joback Method
cpg	343.76	J/molxK	541.83	Joback Method
cpg	361.40	J/molxK	578.98	Joback Method
cpg	377.96	J/molxK	616.14	Joback Method

cpg	393.57	J/mol×K	653.29	Joback Method
cpg	408.36	J/mol×K	690.45	Joback Method
cpg	422.45	J/mol×K	727.60	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=C497621&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C497621&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>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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