

# Bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde, 6,6-dimethyl-

<b>Other names:</b>	2-Norpinene-2-carboxaldehyde, 6,6-dimethyl- Myrtenal Benihinal 6,6-Dimethylbicyclo(3.1.1)hept-2-ene-2-carboxaldehyde 2-Formyl-6,6-dimethylbicyclo(3.1.1)hept-2-ene 6,6-Dimethyl-bicyclo[3,1,1]hept-2-ene-2-carboxaldehyde 6,6-dimethyl-bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde (myrtenal) pin-2-ene-1-carbaldehyde
<b>Inchi:</b>	InChI=1S/C10H14O/c1-10(2)8-4-3-7(6-11)9(10)5-8/h3,6,8-9H,4-5H2,1-2H3
<b>InchiKey:</b>	KMRMUZKLFIEVAO-UHFFFAOYSA-N
<b>Formula:</b>	C10H14O
<b>SMILES:</b>	<chem>CC1(C)C2CC=C(C=O)C1C2</chem>
<b>Mol. weight [g/mol]:</b>	150.22
<b>CAS:</b>	564-94-3

## Physical Properties

Property code	Value	Unit	Source
gf	50.33	kJ/mol	Joback Method
hf	-154.66	kJ/mol	Joback Method
hfus	13.72	kJ/mol	Joback Method
hvap	44.07	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1195.00		NIST Webbook
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tb	493.70	K	NIST Webbook
tc	708.63	K	Joback Method
tf	309.76	K	Joback Method
vc	0.501	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.50	J/mol×K	494.32	Joback Method
cpg	315.43	J/mol×K	530.04	Joback Method
cpg	330.16	J/mol×K	565.76	Joback Method
cpg	343.83	J/mol×K	601.47	Joback Method
cpg	356.59	J/mol×K	637.19	Joback Method
cpg	368.56	J/mol×K	672.91	Joback Method
cpg	379.90	J/mol×K	708.63	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=C564943&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C564943&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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