

# (Z)-«alpha»-Atlantone

<b>Other names:</b>	«alpha»-(Z)-Atlantone
<b>Inchi:</b>	InChI=1S/C15H22O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5,9-10,14H,6-8H2,1-4
<b>InchiKey:</b>	OJEFBZMKKJTKKK-QLKUMGTLA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	CC(C)=CC(=O)C=C(C)C1CC=C(C)CC1
<b>Mol. weight [g/mol]:</b>	218.33
<b>CAS:</b>	56192-70-2

## Physical Properties

Property code	Value	Unit	Source
gf	134.62	kJ/mol	Joback Method
hf	-150.02	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1722.00		NIST Webbook
tb	628.24	K	Joback Method
tc	847.12	K	Joback Method
tf	291.32	K	Joback Method
vc	0.762	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.72	J/molxK	628.24	Joback Method
cpg	541.09	J/molxK	664.72	Joback Method
cpg	559.24	J/molxK	701.20	Joback Method
cpg	576.24	J/molxK	737.68	Joback Method

cpg	592.18	J/mol×K	774.16	Joback Method
cpg	607.10	J/mol×K	810.64	Joback Method
cpg	621.10	J/mol×K	847.12	Joback Method

## Sources

<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=C56192702&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56192702&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>

## 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>mvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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