

# «beta»-Bisabolenal

<b>Inchi:</b>	InChI=1S/C15H22O/c1-12(2)5-4-6-13(3)15-9-7-14(11-16)8-10-15/h5,7,11,15H,3-4,6,8-10
<b>InchiKey:</b>	JZLKKMAUZMMUMS-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	<chem>C=C(CCC=C(C)C)C1CC=C(C=O)CC1</chem>
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	171.64	kJ/mol	Joback Method
hf	-114.81	kJ/mol	Joback Method
hfus	25.86	kJ/mol	Joback Method
hvap	56.53	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1738.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1743.00		NIST Webbook
ripol	2380.00		NIST Webbook
tb	615.55	K	Joback Method
tc	825.26	K	Joback Method
tf	286.71	K	Joback Method
vc	0.774	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.08	J/molxK	615.55	Joback Method
cpg	538.97	J/molxK	650.50	Joback Method
cpg	556.74	J/molxK	685.45	Joback Method
cpg	573.43	J/molxK	720.40	Joback Method
cpg	589.10	J/molxK	755.35	Joback Method
cpg	603.81	J/molxK	790.30	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=R234398&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R234398&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>mccvol:</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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