

# Bisabola-2,6,11-triene

<b>Other names:</b>	Iso-«gamma»-bisabolene
<b>Inchi:</b>	InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h8H,1,5-7,9-11H2,2-4H3/b1
<b>InchiKey:</b>	AAQ GKZZPNFGAFB-CCEZHUSRSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	<chem>C=C(C)CCCC(C)=C1CC=C(C)CC1</chem>
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	244.11	kJ/mol	Joback Method
hf	-50.08	kJ/mol	Joback Method
hfus	22.63	kJ/mol	Joback Method
hvap	50.95	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.179		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	574.04	K	Joback Method
tc	778.59	K	Joback Method
tf	264.39	K	Joback Method
vc	0.761	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.28	J/molxK	574.04	Joback Method
cpg	512.12	J/molxK	608.13	Joback Method
cpg	530.86	J/molxK	642.22	Joback Method
cpg	548.57	J/molxK	676.31	Joback Method
cpg	565.28	J/molxK	710.41	Joback Method
cpg	581.06	J/molxK	744.50	Joback Method
cpg	595.94	J/molxK	778.59	Joback Method

# Sources

<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=R418472&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R418472&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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