

# Bisabolene

**Inchi:** InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6,8,15H,4-5,7,9-11H2,1-3H3  
**InchiKey:** XZRVRYFILCSYSP-UHFFFAOYSA-N  
**Formula:** C15H24  
**SMILES:** C=C(CCC=C(C)C)C1CC=C(C)CC1  
**Mol. weight [g/mol]:** 204.35

## Physical Properties

Property code	Value	Unit	Source
gf	271.16	kJ/mol	Joback Method
hf	-29.23	kJ/mol	Joback Method
hfus	23.58	kJ/mol	Joback Method
hvap	49.81	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1487.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1465.40		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1500.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1736.00		NIST Webbook
ripol	1777.00		NIST Webbook
tb	566.89	K	Joback Method
tc	773.75	K	Joback Method
tf	244.71	K	Joback Method
vc	0.757	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.97	J/mol×K	566.89	Joback Method
cpg	513.94	J/mol×K	601.37	Joback Method
cpg	533.73	J/mol×K	635.84	Joback Method
cpg	552.38	J/mol×K	670.32	Joback Method
cpg	569.95	J/mol×K	704.80	Joback Method
cpg	586.51	J/mol×K	739.28	Joback Method
cpg	602.09	J/mol×K	773.75	Joback Method

## Sources

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R45055&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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