

# «alpha»-Bisabolol

<b>Other names:</b>	Bisabolol 3-Cyclohexene-1-methanol, «alpha»,4-dimethyl-«alpha»-(4-methyl-3-pentenyl)-, (R*,R*)- 5-Hepten-2-ol, 6-methyl-2-(4-methyl-3-cyclohexen-1-yl)- «alpha»,4-Dimethyl-«alpha»-(4-methyl-3-pentenyl)-3-cyclohexene-1-methanol 6-Methyl-2-(4-methyl-3-cyclohexen-1-yl)-5-hepten-2-ol (R*,R*)-«alpha»,4-Dimethyl-«alpha»-(4-methyl-3-pentenyl)-3-cyclohexene-1-methanol (R*,R*)-«alpha»,4-Dimethyl-«alpha»-(4-methyl-3-pentenyl)cyclohex-3-ene-1-methanol 3-Cyclohexene-1-methanol, «alpha»,4-dimethyl-«alpha»-(4-methyl-3-penten-1-yl)- («alpha»,R,1R)-rel- 3-Cyclohexene-1-methanol, «alpha»,4-dimethyl-«alpha»-(4-methyl-3-pentenyl)-, («alpha»,R,1R)-rel- Camfilol Dragosantol Hydagen B dl-«alpha»-Bisabolol «alpha»-bisabolool «alpha»-Bisabalol
<b>Inchi:</b>	InChI=1S/C15H26O/c1-12(2)6-5-11-15(4,16)14-9-7-13(3)8-10-14/h6-7,14,16H,5,8-11H2,
<b>InchiKey:</b>	RGZSQWQPBWRIAQ-CABCVRRESA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	CC(C)=CCCC(C)(O)C1CC=C(C)CC1
<b>Mol. weight [g/mol]:</b>	222.37
<b>CAS:</b>	515-69-5

## Physical Properties

Property code	Value	Unit	Source
gf	57.89	kJ/mol	Joback Method
hf	-305.85	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	65.79	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1668.00		NIST Webbook
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tb	659.28	K	Joback Method
tc	857.10	K	Joback Method
tf	323.67	K	Joback Method
vc	0.783	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.62	J/mol×K	659.28	Joback Method
cpg	607.64	J/mol×K	692.25	Joback Method
cpg	624.61	J/mol×K	725.22	Joback Method
cpg	640.58	J/mol×K	758.19	Joback Method
cpg	655.62	J/mol×K	791.16	Joback Method
cpg	669.79	J/mol×K	824.13	Joback Method
cpg	683.15	J/mol×K	857.10	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C515695&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C515695&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.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>

## 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

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

**vc:** Critical Volume

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