

# Bisabolol oxide B

<b>Other names:</b>	tetrahydro-«alpha», «alpha», 5-trimethyl-5-(4-methyl-3-cyclohexen-1-yl)furan-2-methanol
<b>Inchi:</b>	InChI=1S/C15H26O2/c1-11-5-7-12(8-6-11)15(4)10-9-13(17-15)14(2,3)16/h5,12-13,16H,6
<b>InchiKey:</b>	RKBAYVATPNYHLW-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O2
<b>SMILES:</b>	CC1=CCC(C2(C)CCC(C(C)(C)O)O2)CC1
<b>Mol. weight [g/mol]:</b>	238.37
<b>CAS:</b>	55399-12-7

## Physical Properties

Property code	Value	Unit	Source
gf	-76.55	kJ/mol	Joback Method
hf	-489.90	kJ/mol	Joback Method
hfus	20.64	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.441		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1636.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
tb	693.04	K	Joback Method
tc	909.66	K	Joback Method
tf	399.84	K	Joback Method
vc	0.761	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.37	J/mol×K	693.04	Joback Method
cpg	655.24	J/mol×K	729.14	Joback Method
cpg	674.05	J/mol×K	765.25	Joback Method
cpg	691.94	J/mol×K	801.35	Joback Method
cpg	709.08	J/mol×K	837.46	Joback Method
cpg	725.60	J/mol×K	873.56	Joback Method
cpg	741.67	J/mol×K	909.66	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=C55399127&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55399127&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

**vc:** Critical Volume

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