

# Bisabolone (6S,7R)

<b>Inchi:</b>	InChI=1S/C15H24O/c1-11(2)6-5-7-13(4)14-9-8-12(3)10-15(14)16/h6,10,13-14H,5,7-9H2,
<b>InchiKey:</b>	KNOUERLLBMJGLF-LSLKUGRBSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC(C)=CCCC(C)C1CCC(C)=CC1=O
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	66.84	kJ/mol	Joback Method
hf	-287.85	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.294		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1745.00		NIST Webbook
tb	637.71	K	Joback Method
tc	853.69	K	Joback Method
tf	313.65	K	Joback Method
vc	0.776	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.22	J/molxK	637.71	Joback Method
cpg	575.88	J/molxK	673.71	Joback Method
cpg	595.37	J/molxK	709.70	Joback Method
cpg	613.70	J/molxK	745.70	Joback Method
cpg	630.91	J/molxK	781.70	Joback Method
cpg	647.03	J/molxK	817.69	Joback Method
cpg	662.08	J/molxK	853.69	Joback Method

# Sources

<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=R626678&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R626678&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>rinpola:</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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