

# «beta»-helmiscapene

<b>Inchi:</b>	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h13-14H,1,3,5-10H2,2,4
<b>InchiKey:</b>	YOVSPTNQHMDJAG-LOWNFYCTSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	<chem>C=C(C)C1CCC2(C)CCCC(=C)C2C1</chem>
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	267.69	kJ/mol	Joback Method
hf	-37.19	kJ/mol	Joback Method
hfus	13.50	kJ/mol	Joback Method
hvap	47.61	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1446.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1686.00		NIST Webbook
tb	564.45	K	Joback Method
tc	788.06	K	Joback Method
tf	298.23	K	Joback Method
vc	0.721	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.99	J/mol×K	564.45	Joback Method
cpg	521.74	J/mol×K	601.72	Joback Method
cpg	543.99	J/mol×K	638.99	Joback Method

cpg	564.88	J/mol×K	676.25	Joback Method
cpg	584.58	J/mol×K	713.52	Joback Method
cpg	603.25	J/mol×K	750.79	Joback Method
cpg	621.03	J/mol×K	788.06	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=R141716&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R141716&amp;Units=SI</a>
<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>

## 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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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