

# «beta»-Betulenal

<b>Other names:</b>	Isocaryophyllen-14-al («beta»-Betulenal)
<b>Inchi:</b>	InChI=1S/C15H22O/c1-11-5-4-6-12(10-16)7-8-14-13(11)9-15(14,2)3/h6,10,13-14H,1,4-5
<b>InchiKey:</b>	PDGJMGSNVOPQRK-SDQBPNPISA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	<chem>C=C1CCC=C(C=O)CCC2C1CC2(C)C</chem>
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	97.11	kJ/mol	Joback Method
hf	-198.26	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	56.04	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
ripol	2193.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2193.00		NIST Webbook
tb	624.96	K	Joback Method
tc	852.75	K	Joback Method
tf	365.71	K	Joback Method
vc	0.734	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.57	J/mol×K	624.96	Joback Method
cpg	550.73	J/mol×K	662.92	Joback Method

cpg	570.64	J/mol×K	700.89	Joback Method
cpg	589.44	J/mol×K	738.85	Joback Method
cpg	607.27	J/mol×K	776.82	Joback Method
cpg	624.28	J/mol×K	814.78	Joback Method
cpg	640.60	J/mol×K	852.75	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=R336102&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R336102&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>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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