

# «beta»-Caryophyllene, 14-oxy

<b>Inchi:</b>	InChI=1S/C15H24O/c1-11-5-4-6-12(10-16)7-8-14-13(11)9-15(14,2)3/h6,13-14,16H,1,4-5
<b>InchiKey:</b>	MGIQTXDHQJGPEZ-DCOFTTSXSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>C=C1CCC=C(CO)CCC2C1CC2(C)C</chem>
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	59.81	kJ/mol	Joback Method
hf	-264.91	kJ/mol	Joback Method
hfus	18.91	kJ/mol	Joback Method
hvap	66.00	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
ripol	2357.00		NIST Webbook
tb	668.48	K	Joback Method
tc	877.54	K	Joback Method
tf	384.53	K	Joback Method
vc	0.736	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.23	J/mol×K	668.48	Joback Method
cpg	593.26	J/mol×K	703.32	Joback Method
cpg	611.33	J/mol×K	738.17	Joback Method
cpg	628.56	J/mol×K	773.01	Joback Method
cpg	645.05	J/mol×K	807.85	Joback Method
cpg	660.93	J/mol×K	842.69	Joback Method
cpg	676.30	J/mol×K	877.54	Joback Method

# Sources

<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=R410389&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R410389&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>
<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>

# 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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