

# Caryophylla-4(14),8(15)-dien-5-one

<b>Inchi:</b>	InChI=1S/C15H24O/c1-12-7-8-14(16)13(2)6-5-10-15(3,4)11-9-12/h1-2,5-11H2,3-4H3
<b>InchiKey:</b>	UKHXWJYIXLAHEV-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>C=C1CCC(=O)C(=C)CCCC(C)(C)CC1</chem>
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	17.45	kJ/mol	Joback Method
hf	-283.39	kJ/mol	Joback Method
hfus	6.83	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.438		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinqol	1559.00		NIST Webbook
tb	649.88	K	Joback Method
tc	894.53	K	Joback Method
tf	368.07	K	Joback Method
vc	0.742	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.07	J/mol×K	649.88	Joback Method
cpg	585.57	J/mol×K	690.65	Joback Method
cpg	608.65	J/mol×K	731.43	Joback Method
cpg	630.37	J/mol×K	772.20	Joback Method
cpg	650.81	J/mol×K	812.98	Joback Method
cpg	670.02	J/mol×K	853.75	Joback Method
cpg	688.07	J/mol×K	894.53	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=R227340&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R227340&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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