

# Caryophylla-3(15),7(14)-dien-6-one

<b>Inchi:</b>	InChI=1S/C15H22O/c1-10-5-7-13-12(9-15(13,3)4)11(2)14(16)8-6-10/h12-13H,1-2,5-9H2
<b>InchiKey:</b>	NZPOBSKADKAQSR-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	<chem>C=C1CCC(=O)C(=C)C2CC(C)(C)C2CC1</chem>
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	106.79	kJ/mol	Joback Method
hf	-212.45	kJ/mol	Joback Method
hfus	12.34	kJ/mol	Joback Method
hvap	52.78	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinqol	1563.00		NIST Webbook
tb	639.14	K	Joback Method
tc	876.58	K	Joback Method
tf	392.33	K	Joback Method
vc	0.722	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.15	J/mol×K	639.14	Joback Method
cpg	563.82	J/mol×K	678.71	Joback Method
cpg	585.20	J/mol×K	718.29	Joback Method
cpg	605.43	J/mol×K	757.86	Joback Method
cpg	624.62	J/mol×K	797.43	Joback Method
cpg	642.88	J/mol×K	837.00	Joback Method
cpg	660.33	J/mol×K	876.58	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=R231200&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R231200&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>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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