

# Caryophyllane-a

<b>Inchi:</b>	InChI=1S/C15H28/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/h11-14H,5-10H2,1-4H3
<b>InchiKey:</b>	SITKOPDZOGHVLY-UHFFFAOYSA-N
<b>Formula:</b>	C15H28
<b>SMILES:</b>	CC1CCCC(C)C2CC(C)(C)C2CC1
<b>Mol. weight [g/mol]:</b>	208.38

## Physical Properties

Property code	Value	Unit	Source
gf	107.80	kJ/mol	Joback Method
hf	-283.91	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	47.59	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.885		Crippen Method
mcvol	200.490	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1425.00		NIST Webbook
rinpol	1425.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1522.00		NIST Webbook
tb	563.66	K	Joback Method
tc	784.20	K	Joback Method
tf	288.27	K	Joback Method
vc	0.745	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.83	J/molxK	563.66	Joback Method
cpg	569.05	J/molxK	600.42	Joback Method
cpg	594.68	J/molxK	637.17	Joback Method
cpg	618.83	J/molxK	673.93	Joback Method
cpg	641.64	J/molxK	710.68	Joback Method
cpg	663.22	J/molxK	747.44	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=R306517&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R306517&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>mccvol:</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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