

# (+)(-)-(E)-«beta»-caryophyllene

<b>Inchi:</b>	InChI=1S/C15H24/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/h13-14H,1-2,5-10H2,3-4
<b>InchiKey:</b>	PMMLIVYPEUJENN-KBPBESRZSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	<chem>C=C1CCCC(=C)C2CC(C)(C)C2CC1</chem>
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	229.38	kJ/mol	Joback Method
hf	-74.75	kJ/mol	Joback Method
hfus	12.83	kJ/mol	Joback Method
hvap	48.53	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
tb	571.32	K	Joback Method
tc	795.83	K	Joback Method
tf	324.11	K	Joback Method
vc	0.715	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.15	J/mol×K	571.32	Joback Method
cpg	523.89	J/mol×K	608.74	Joback Method
cpg	546.20	J/mol×K	646.16	Joback Method
cpg	567.20	J/mol×K	683.57	Joback Method
cpg	587.05	J/mol×K	720.99	Joback Method
cpg	605.87	J/mol×K	758.41	Joback Method
cpg	623.79	J/mol×K	795.83	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=R504008&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R504008&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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