

# «delta»-Guajene

<b>Inchi:</b>	InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h12-13,15H,1,5-9H2,2-4
<b>InchiKey:</b>	YHAJBLWYOIUHHM-GZBFAFLISA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	<chem>C=C(C)C1CCC(C)=C2CCC(C)C2C1</chem>
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	230.80	kJ/mol	Joback Method
hf	-101.83	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinsol	1495.00		NIST Webbook
tb	574.17	K	Joback Method
tc	791.30	K	Joback Method
tf	286.45	K	Joback Method
vc	0.725	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.80	J/mol×K	574.17	Joback Method
cpg	525.03	J/mol×K	610.36	Joback Method
cpg	546.90	J/mol×K	646.55	Joback Method
cpg	567.47	J/mol×K	682.74	Joback Method
cpg	586.78	J/mol×K	718.92	Joback Method
cpg	604.90	J/mol×K	755.11	Joback Method
cpg	621.88	J/mol×K	791.30	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R610252&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R610252&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>
<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>

# 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>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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