

# Gurjunene

<b>Inchi:</b>	InChI=1S/C15H24/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h9,11-12,14H,5-8H2,1
<b>InchiKey:</b>	SPCXZDDGSGTVAW-XIDUGBJDSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	CC1=C2C(CC1)C(C)CCC1C2C1(C)C
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	223.26	kJ/mol	Joback Method
hf	-137.45	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	48.91	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinqol	1475.00		NIST Webbook
tb	571.38	K	Joback Method
tc	789.11	K	Joback Method
tf	346.81	K	Joback Method
vc	0.713	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.59	J/molxK	571.38	Joback Method
cpg	528.29	J/molxK	607.67	Joback Method
cpg	549.58	J/molxK	643.96	Joback Method
cpg	569.63	J/molxK	680.24	Joback Method
cpg	588.60	J/molxK	716.53	Joback Method
cpg	606.66	J/molxK	752.82	Joback Method
cpg	624.00	J/molxK	789.11	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=R520015&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R520015&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>

# 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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