

# «gamma»-Gurjunene epoxide

<b>Inchi:</b>	InChI=1S/C15H26O/c1-9(2)12-7-5-10(3)13-8-6-11(4)15(13)14(12)16-15/h9-14H,5-8H2,1
<b>InchiKey:</b>	YWPRRALOHVWEQD-MNTSOTEJSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	CC(C)C1CCC(C)C2CCC(C)C23OC13
<b>Mol. weight [g/mol]:</b>	222.37

## Physical Properties

Property code	Value	Unit	Source
gf	116.29	kJ/mol	Joback Method
hf	-329.91	kJ/mol	Joback Method
hfus	26.18	kJ/mol	Joback Method
hvap	51.11	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.872		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	1542.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1542.00		NIST Webbook
tb	584.10	K	Joback Method
tc	800.18	K	Joback Method
tf	328.34	K	Joback Method
vc	0.741	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.45	J/mol×K	584.10	Joback Method
cpg	585.76	J/mol×K	620.11	Joback Method
cpg	608.55	J/mol×K	656.13	Joback Method
cpg	630.00	J/mol×K	692.14	Joback Method
cpg	650.29	J/mol×K	728.16	Joback Method
cpg	669.59	J/mol×K	764.17	Joback Method
cpg	688.05	J/mol×K	800.18	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=R439959&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R439959&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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