

# «beta»-Spathulene

<b>Inchi:</b>	InChI=1S/C15H22/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h11-14H,1-2,5-8H2,3-4H
<b>InchiKey:</b>	JNXBLAGJPYZBMG-REWJHTLYSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	<chem>C=C1CCC2C(C3C(=C)CCC13)C2(C)C</chem>
<b>Mol. weight [g/mol]:</b>	202.34

## Physical Properties

Property code	Value	Unit	Source
gf	318.72	kJ/mol	Joback Method
hf	-3.81	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	47.62	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.191		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinqol	1452.00		NIST Webbook
tb	560.58	K	Joback Method
tc	777.89	K	Joback Method
tf	348.37	K	Joback Method
vc	0.695	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.79	J/mol×K	560.58	Joback Method
cpg	504.87	J/mol×K	596.80	Joback Method
cpg	525.53	J/mol×K	633.02	Joback Method
cpg	544.93	J/mol×K	669.23	Joback Method
cpg	563.24	J/mol×K	705.45	Joback Method
cpg	580.63	J/mol×K	741.67	Joback Method
cpg	597.27	J/mol×K	777.89	Joback Method

# Sources

<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=R604905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R604905&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>

# 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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