

# Bourbonene

<b>Inchi:</b>	InChI=1S/C15H24/c1-9(2)11-7-8-15(4)12-6-5-10(3)13(12)14(11)15/h9,11-14H,3,5-8H2,1
<b>InchiKey:</b>	YIRAHEODBQONHI-UHFFFAOYSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	C=C1CCC2C1C1C(C(C)C)CCC21C
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	275.30	kJ/mol	Joback Method
hf	-87.17	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
ripol	1531.00		NIST Webbook
tb	556.71	K	Joback Method
tc	769.30	K	Joback Method
tf	323.21	K	Joback Method
vc	0.713	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.63	J/molxK	556.71	Joback Method
cpg	524.39	J/molxK	592.14	Joback Method
cpg	545.67	J/molxK	627.57	Joback Method
cpg	565.65	J/molxK	663.00	Joback Method
cpg	584.49	J/molxK	698.44	Joback Method
cpg	602.37	J/molxK	733.87	Joback Method
cpg	619.46	J/molxK	769.30	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=R283444&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R283444&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>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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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