

# Isobazzanene

**Inchi:** InChI=1S/C15H24/c1-12-7-10-15(4,11-8-12)13-6-5-9-14(13,2)3/h6-7H,5,8-11H2,1-4H3/t1  
**InchiKey:** WUOZOSFJWTXTKG-OAHLLOKOSA-N  
**Formula:** C15H24  
**SMILES:** CC1=CCC(C)(C2=CCCC2(C)C)CC1  
**Mol. weight [g/mol]:** 204.35

## Physical Properties

Property code	Value	Unit	Source
gf	166.10	kJ/mol	Joback Method
hf	-115.03	kJ/mol	Joback Method
hfus	9.45	kJ/mol	Joback Method
hvap	49.28	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpola	1442.00		NIST Webbook
rinpola	1442.00		NIST Webbook
tb	586.19	K	Joback Method
tc	822.53	K	Joback Method
tf	351.45	K	Joback Method
vc	0.718	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.78	J/mol×K	586.19	Joback Method
cpg	523.43	J/mol×K	625.58	Joback Method
cpg	544.65	J/mol×K	664.97	Joback Method
cpg	564.73	J/mol×K	704.36	Joback Method
cpg	583.94	J/mol×K	743.75	Joback Method
cpg	602.58	J/mol×K	783.14	Joback Method
cpg	620.93	J/mol×K	822.53	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=R424170&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R424170&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>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>rinpola:</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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