

# iso-«beta»-elemene

<b>Inchi:</b>	InChI=1S/C15H24/c1-7-15(6)10-8-9-13(11(2)3)14(15)12(4)5/h7,13-14H,1-2,4,8-10H2,3,5
<b>InchiKey:</b>	GJWVPRIGTFVAQW-RBSFLKMASA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	<chem>C=CC1(C)CCCC(C(=C)C)C1C(=C)C</chem>
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	325.38	kJ/mol	Joback Method
hf	32.66	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	45.79	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.747		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinqol	1379.00		NIST Webbook
tb	542.85	K	Joback Method
tc	754.13	K	Joback Method
tf	248.41	K	Joback Method
vc	0.750	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.78	J/mol×K	542.85	Joback Method
cpg	511.42	J/mol×K	578.06	Joback Method
cpg	532.71	J/mol×K	613.28	Joback Method
cpg	552.77	J/mol×K	648.49	Joback Method
cpg	571.73	J/mol×K	683.70	Joback Method
cpg	589.70	J/mol×K	718.92	Joback Method
cpg	606.82	J/mol×K	754.13	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=R340542&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R340542&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.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>

# 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>mccvol:</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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