

# «beta»-Elemen-9-«beta»-ol

<b>Inchi:</b>	InChI=1S/C15H24O/c1-7-15(6)13(11(4)5)8-12(10(2)3)9-14(15)16/h7,12-14,16H,1-2,4,8-9
<b>InchiKey:</b>	YFNGGCSSPZBZRN-TUVASFSCSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	C=CC1(C)C(O)CC(C(=C)C)CC1C(=C)C
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	180.85	kJ/mol	Joback Method
hf	-139.91	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	62.16	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.718		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
ripol	2018.00		NIST Webbook
ripol	2018.00		NIST Webbook
tb	630.36	K	Joback Method
tc	827.75	K	Joback Method
tf	304.99	K	Joback Method
vc	0.767	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.87	J/mol×K	630.36	Joback Method
cpg	582.68	J/mol×K	663.26	Joback Method
cpg	600.55	J/mol×K	696.16	Joback Method
cpg	617.57	J/mol×K	729.06	Joback Method
cpg	633.84	J/mol×K	761.95	Joback Method
cpg	649.46	J/mol×K	794.85	Joback Method
cpg	664.52	J/mol×K	827.75	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=R238518&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R238518&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>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>ri pol:</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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