

# Isocedranol

<b>Inchi:</b>	InChI=1S/C15H26O/c1-10-5-6-11-13(2,3)12-9-15(10,11)8-7-14(12,4)16/h10-12,16H,5-9H
<b>InchiKey:</b>	SVURIXNDRWRAFU-IVGFHQPOSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	CC1CCC2C(C)(C)C3CC12CCC3(C)O
<b>Mol. weight [g/mol]:</b>	222.37

## Physical Properties

Property code	Value	Unit	Source
gf	57.05	kJ/mol	Joback Method
hf	-314.38	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	61.37	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.610		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinqol	1669.00		NIST Webbook
tb	650.25	K	Joback Method
tc	863.66	K	Joback Method
tf	425.39	K	Joback Method
vc	0.741	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.75	J/molxK	650.25	Joback Method
cpg	615.74	J/molxK	685.82	Joback Method
cpg	634.97	J/molxK	721.39	Joback Method
cpg	653.76	J/molxK	756.96	Joback Method
cpg	672.45	J/molxK	792.52	Joback Method
cpg	691.37	J/molxK	828.09	Joback Method
cpg	710.84	J/molxK	863.66	Joback Method

# Sources

<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>
<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=R338757&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R338757&amp;Units=SI</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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