

# (E)-Isovalencenal

## [eremophila-1(10),7(11)-dien-12-al

Inchi:	InChI=1S/C15H22O/c1-11(10-16)13-7-8-14-6-4-5-12(2)15(14,3)9-13/h6,10,12H,4-5,7-9H
InchiKey:	SVFQWLHYXVFRHQ-NVXNZCMISA-N
Formula:	C15H22O
SMILES:	CC(C=O)=C1CCC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]:	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	100.75	kJ/mol	Joback Method
hf	-189.76	kJ/mol	Joback Method
hfus	18.31	kJ/mol	Joback Method
hvap	56.89	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rmpol	1800.00		NIST Webbook
tb	632.72	K	Joback Method
tc	861.77	K	Joback Method
tf	356.19	K	Joback Method
vc	0.743	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.12	J/mol×K	632.72	Joback Method
cpg	547.19	J/mol×K	670.90	Joback Method
cpg	566.08	J/mol×K	709.07	Joback Method
cpg	583.95	J/mol×K	747.25	Joback Method
cpg	600.97	J/mol×K	785.42	Joback Method
cpg	617.33	J/mol×K	823.60	Joback Method
cpg	633.20	J/mol×K	861.77	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=R397890&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R397890&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>hvac:</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>mccol:</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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