

# (-)-Elema-1,3,11(13)-trien-12-ol

<b>Inchi:</b>	InChI=1S/C15H24O/c1-6-15(5)8-7-13(12(4)10-16)9-14(15)11(2)3/h6,13-14,16H,1-2,4,7-11H
<b>InchiKey:</b>	KNLJFYVIVVSUNJ-ZNMIVQPWSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	C=CC1(C)CCC(C(=C)CO)CC1C(=C)C
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	188.56	kJ/mol	Joback Method
hf	-119.57	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.720		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
tb	635.03	K	Joback Method
tc	832.55	K	Joback Method
tf	309.23	K	Joback Method
vc	0.768	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.36	J/mol×K	635.03	Joback Method
cpg	580.72	J/mol×K	667.95	Joback Method
cpg	598.15	J/mol×K	700.87	Joback Method
cpg	614.76	J/mol×K	733.79	Joback Method
cpg	630.64	J/mol×K	766.71	Joback Method
cpg	645.91	J/mol×K	799.63	Joback Method
cpg	660.66	J/mol×K	832.55	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=R336731&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R336731&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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