

# epi-«alpha»-Elemol

<b>Inchi:</b>	InChI=1S/C15H26O/c1-7-15(6)9-8-12(14(4,5)16)10-13(15)11(2)3/h7,12-13,16H,1-2,8-10
<b>InchiKey:</b>	GFJIQNADMLPFOW-NFAWXSAZSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	<chem>C=CC1(C)CCC(C(C)(C)O)CC1C(=C)C</chem>
<b>Mol. weight [g/mol]:</b>	222.37

## Physical Properties

Property code	Value	Unit	Source
gf	112.11	kJ/mol	Joback Method
hf	-243.96	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	61.77	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.942		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinsol	1625.00		NIST Webbook
tb	635.24	K	Joback Method
tc	836.45	K	Joback Method
tf	327.37	K	Joback Method
vc	0.775	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.75	J/mol×K	635.24	Joback Method
cpg	607.17	J/mol×K	668.78	Joback Method
cpg	625.55	J/mol×K	702.31	Joback Method
cpg	642.99	J/mol×K	735.85	Joback Method
cpg	659.62	J/mol×K	769.38	Joback Method
cpg	675.56	J/mol×K	802.92	Joback Method
cpg	690.93	J/mol×K	836.45	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=R412058&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R412058&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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