

# Isolongifolene, 9,10-dehydro-

<b>Other names:</b>	9,10-Dehydroisolongifolene
<b>Inchi:</b>	InChI=1S/C15H22/c1-13(2)8-5-6-12-14(3,4)11-7-9-15(12,13)10-11/h5-6,8,11H,7,9-10H2,
<b>InchiKey:</b>	UIPKEVNEOFKIRG-UHFFFAOYSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	CC1(C)C2=CC=CC(C)(C)C23CCC1C3
<b>Mol. weight [g/mol]:</b>	202.34

## Physical Properties

Property code	Value	Unit	Source
gf	259.58	kJ/mol	Joback Method
hf	-17.38	kJ/mol	Joback Method
hfus	9.04	kJ/mol	Joback Method
hvap	46.55	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
ripol	1913.00		NIST Webbook
ripol	1913.00		NIST Webbook
tb	570.71	K	Joback Method
tc	808.01	K	Joback Method
tf	387.09	K	Joback Method
vc	0.696	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.77	J/mol×K	570.71	Joback Method
cpg	502.91	J/mol×K	610.26	Joback Method
cpg	522.45	J/mol×K	649.81	Joback Method
cpg	540.85	J/mol×K	689.36	Joback Method
cpg	558.58	J/mol×K	728.91	Joback Method
cpg	576.10	J/mol×K	768.46	Joback Method
cpg	593.88	J/mol×K	808.01	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=U151671&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U151671&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>ripol:</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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