

# «alpha»-Cuprenene

<b>Inchi:</b>	InChI=1S/C15H24/c1-12-6-8-13(9-7-12)15(4)11-5-10-14(15,2)3/h6,8H,5,7,9-11H2,1-4H3
<b>InchiKey:</b>	DYQFFTPJVWEYMH-UHFFFAOYSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	CC1=CC=C(C2(C)CCCC2(C)C)CC1
<b>Mol. weight [g/mol]:</b>	204.35
<b>CAS:</b>	29621-78-1

## Physical Properties

Property code	Value	Unit	Source
gf	166.10	kJ/mol	Joback Method
hf	-115.03	kJ/mol	Joback Method
hfus	9.45	kJ/mol	Joback Method
hvap	49.28	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1497.00		NIST Webbook
rinpol	1513.60		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1513.60		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1504.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1759.00		NIST Webbook
tb	586.19	K	Joback Method
tc	822.53	K	Joback Method
tf	351.45	K	Joback Method
vc	0.718	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.78	J/mol×K	586.19	Joback Method
cpg	523.43	J/mol×K	625.58	Joback Method
cpg	544.65	J/mol×K	664.97	Joback Method
cpg	564.73	J/mol×K	704.36	Joback Method
cpg	583.94	J/mol×K	743.75	Joback Method
cpg	602.58	J/mol×K	783.14	Joback Method
cpg	620.93	J/mol×K	822.53	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C29621781&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29621781&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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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