

# «alpha»-Neocallitropsene

<b>Inchi:</b>	InChI=1S/C15H26/c1-11(2)14-6-5-13(4)15(14)9-7-12(3)8-10-15/h7,11,13-14H,5-6,8-10H
<b>InchiKey:</b>	OHMAJNDAPNNXHC-ZYOSVBKOSA-N
<b>Formula:</b>	C15H26
<b>SMILES:</b>	CC1=CCC2(CC1)C(C)CCC2C(C)C
<b>Mol. weight [g/mol]:</b>	206.37

## Physical Properties

Property code	Value	Unit	Source
gf	153.21	kJ/mol	Joback Method
hf	-196.04	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	48.60	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.805		Crippen Method
mcvol	196.190	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1477.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1485.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1695.00		NIST Webbook
tb	572.43	K	Joback Method
tc	793.31	K	Joback Method
tf	298.55	K	Joback Method
vc	0.735	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	521.00	J/mol×K	572.43	Joback Method
cpg	545.14	J/mol×K	609.24	Joback Method
cpg	567.82	J/mol×K	646.06	Joback Method
cpg	589.17	J/mol×K	682.87	Joback Method
cpg	609.34	J/mol×K	719.68	Joback Method
cpg	628.49	J/mol×K	756.50	Joback Method
cpg	646.76	J/mol×K	793.31	Joback Method

## Sources

<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=R339978&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R339978&amp;Units=SI</a>
<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>

## 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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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