

# 3-Cadinene

<b>Inchi:</b>	InChI=1S/C15H26/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,10,12-15H,6-9H2,1-4H
<b>InchiKey:</b>	IHQBZSSZQWCOOB-IBLUKRHDSA-N
<b>Formula:</b>	C15H26
<b>SMILES:</b>	CC1=CCC2C(C)CCC(C(C)C)C2C1
<b>Mol. weight [g/mol]:</b>	206.37

## Physical Properties

Property code	Value	Unit	Source
gf	150.99	kJ/mol	Joback Method
hf	-231.62	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	49.45	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.661		Crippen Method
mvol	196.190	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	1511.00		NIST Webbook
rinpol	1511.00		NIST Webbook
tb	567.52	K	Joback Method
tc	779.81	K	Joback Method
tf	270.41	K	Joback Method
vc	0.736	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.65	J/molxK	567.52	Joback Method
cpg	547.31	J/molxK	602.90	Joback Method
cpg	570.58	J/molxK	638.28	Joback Method
cpg	592.50	J/molxK	673.67	Joback Method
cpg	613.13	J/molxK	709.05	Joback Method
cpg	632.50	J/molxK	744.43	Joback Method
cpg	650.67	J/molxK	779.81	Joback Method
dvisc	0.0023277	Paxs	270.41	Joback Method

dvisc	0.0013591	Paxs	319.93	Joback Method
dvisc	0.0009166	Paxs	369.45	Joback Method
dvisc	0.0006786	Paxs	418.96	Joback Method
dvisc	0.0005353	Paxs	468.48	Joback Method
dvisc	0.0004419	Paxs	518.00	Joback Method
dvisc	0.0003771	Paxs	567.52	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=R205300&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R205300&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>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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