

# «sigma»-Cadinene

<b>Inchi:</b>	InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h9-10,13,15H,5-8H2,1-4H
<b>InchiKey:</b>	FUCYIEXQVQJBKY-ZFWWWQNUSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	CC1=CC2C(=C(C)CCC2C(C)C)CC1
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	177.11	kJ/mol	Joback Method
hf	-156.10	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1524.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1530.50		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1523.00		NIST Webbook
ripol	1749.00		NIST Webbook
tb	585.98	K	Joback Method
tc	802.43	K	Joback Method
tf	304.69	K	Joback Method
vc	0.724	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.23	J/molxK	585.98	Joback Method
cpg	525.21	J/molxK	622.06	Joback Method
cpg	545.92	J/molxK	658.13	Joback Method
cpg	565.40	J/molxK	694.21	Joback Method

cpg	583.72	J/mol×K	730.28	Joback Method
cpg	600.91	J/mol×K	766.36	Joback Method
cpg	617.03	J/mol×K	802.43	Joback Method
dvisc	0.0020981	Paxs	304.69	Joback Method
dvisc	0.0012209	Paxs	351.57	Joback Method
dvisc	0.0008070	Paxs	398.45	Joback Method
dvisc	0.0005820	Paxs	445.34	Joback Method
dvisc	0.0004467	Paxs	492.22	Joback Method
dvisc	0.0003590	Paxs	539.10	Joback Method
dvisc	0.0002988	Paxs	585.98	Joback Method

## Sources

<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=R281493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R281493&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>
<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>

## 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>mvol:</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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