

# cis,trans,cis-2-Ethyl-1,3-dimethylcyclopentane

Inchi:	InChI=1S/C9H18/c1-4-9-7(2)5-6-8(9)3/h7-9H,4-6H2,1-3H3/t7-,8+,9+
InchiKey:	JREISGVVJTVFBL-BRPSZJMVSA-N
Formula:	C9H18
SMILES:	CCC1C(C)CCC1C
Mol. weight [g/mol]:	126.24

## Physical Properties

Property code	Value	Unit	Source
gf	46.03	kJ/mol	Joback Method
hf	-209.29	kJ/mol	Joback Method
hfus	15.14	kJ/mol	Joback Method
hvap	35.27	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	846.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	844.00		NIST Webbook
tb	411.26	K	Joback Method
tc	601.43	K	Joback Method
tf	193.61	K	Joback Method
vc	0.478	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.59	J/molxK	411.26	Joback Method
cpg	273.61	J/molxK	442.96	Joback Method
cpg	290.88	J/molxK	474.65	Joback Method
cpg	307.41	J/molxK	506.35	Joback Method

cpg	323.20	J/molxK	538.04	Joback Method
cpg	338.29	J/molxK	569.74	Joback Method
cpg	352.67	J/molxK	601.43	Joback Method
dvisc	0.0013588	Paxs	193.61	Joback Method
dvisc	0.0008515	Paxs	229.89	Joback Method
dvisc	0.0006061	Paxs	266.16	Joback Method
dvisc	0.0004681	Paxs	302.44	Joback Method
dvisc	0.0003821	Paxs	338.71	Joback Method
dvisc	0.0003244	Paxs	374.99	Joback Method
dvisc	0.0002834	Paxs	411.26	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R92933&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R92933&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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