

# 1-[(E)-1,4,7,10,11,14,15-heptamethyl-4-vinyl-5-hex

InChI: **Isomer # 2** InChI=1S/C34H64/c1-13-34(12,23-21-30(8)32-19-18-31(9)33(10,11)24-32)22-20-26(4)14  
InChIKey: MXZICHDKCVIUPH-LSDHQDQOSA-N

Formula: C34H64

SMILES: C=CC(C)(C=CC(C)CCC(C)C(C)CCC(C)C(C)C)CCC(C)C1CCC(C)C(C)(C)C1

Mol. weight [g/mol]: 472.87

## Physical Properties

Property code	Value	Unit	Source
gf	395.20	kJ/mol	Joback Method
hf	-513.99	kJ/mol	Joback Method
hfus	41.86	kJ/mol	Joback Method
hvap	85.60	kJ/mol	Joback Method
log10ws	-11.24		Crippen Method
logp	11.374		Crippen Method
mcvol	470.460	ml/mol	McGowan Method
pc	584.29	kPa	Joback Method
rinpol	2771.00		NIST Webbook
rinpol	2771.00		NIST Webbook
tb	982.74	K	Joback Method
tc	1203.15	K	Joback Method
tf	401.32	K	Joback Method
vc	1.782	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1710.18	J/molxK	982.74	Joback Method
cpg	1740.97	J/molxK	1019.47	Joback Method
cpg	1771.10	J/molxK	1056.21	Joback Method
cpg	1800.79	J/molxK	1092.94	Joback Method
cpg	1830.28	J/molxK	1129.68	Joback Method
cpg	1859.80	J/molxK	1166.41	Joback Method
cpg	1889.59	J/molxK	1203.15	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=R586411&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R586411&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>rinpola:</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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