

# C34 17A,21B,22R-Hopane

<b>Inchi:</b>	InChI=1S/C34H60/c1-9-10-11-13-24(2)25-16-21-31(5)26(25)17-22-33(7)28(31)14-15-29
<b>InchiKey:</b>	BFOUVXJORMEENT-ADARNOGESA-N
<b>Formula:</b>	C34H60
<b>SMILES:</b>	CCCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
<b>Mol. weight [g/mol]:</b>	468.84

## Physical Properties

Property code	Value	Unit	Source
gf	398.11	kJ/mol	Joback Method
hf	-448.83	kJ/mol	Joback Method
hfus	32.23	kJ/mol	Joback Method
hvap	84.19	kJ/mol	Joback Method
log10ws	-10.87		Crippen Method
logp	10.694		Crippen Method
mcvol	435.620	ml/mol	McGowan Method
pc	765.64	kPa	Joback Method
rinsol	3535.00		NIST Webbook
tb	1014.05	K	Joback Method
tc	1252.75	K	Joback Method
tf	624.82	K	Joback Method
vc	1.655	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1772.68	J/molxK	1014.05	Joback Method
cpg	1830.40	J/molxK	1053.83	Joback Method
cpg	1892.78	J/molxK	1093.62	Joback Method
cpg	1960.59	J/molxK	1133.40	Joback Method
cpg	2034.62	J/molxK	1173.18	Joback Method
cpg	2115.64	J/molxK	1212.96	Joback Method
cpg	2204.43	J/molxK	1252.75	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=R56339&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R56339&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>mccvol:</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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