

# C33-Hopane, 17bH, 21aH, 22RS

**Inchi:** InChI=1S/C33H58/c1-9-10-12-23(2)24-15-20-30(5)25(24)16-21-32(7)27(30)13-14-28-31  
**InchiKey:** KTWXNNDHFXEEFL-LVICMRJYSA-N  
**Formula:** C33H58  
**SMILES:** CCCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C  
**Mol. weight [g/mol]:** 454.81

## Physical Properties

Property code	Value	Unit	Source
gf	389.69	kJ/mol	Joback Method
hf	-428.19	kJ/mol	Joback Method
hfus	29.64	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-10.45		Crippen Method
logp	10.304		Crippen Method
mvol	421.530	ml/mol	McGowan Method
pc	807.99	kPa	Joback Method
rinpol	3395.00		NIST Webbook
rinpol	3395.00		NIST Webbook
tb	991.17	K	Joback Method
tc	1229.95	K	Joback Method
tf	613.55	K	Joback Method
vc	1.599	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1689.90	J/molxK	991.17	Joback Method
cpg	1744.45	J/molxK	1030.97	Joback Method
cpg	1803.28	J/molxK	1070.76	Joback Method
cpg	1867.15	J/molxK	1110.56	Joback Method
cpg	1936.84	J/molxK	1150.35	Joback Method
cpg	2013.12	J/molxK	1190.15	Joback Method
cpg	2096.77	J/molxK	1229.95	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R553689&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R553689&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>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>hvp:</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>rinp:</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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