

# C32-25-Norhopane, 17aH, 21bH, 22S

**Inchi:** InChI=1S/C31H54/c1-8-10-21(2)22-14-18-29(5)25(22)16-20-31(7)27(29)13-12-26-23-11-10  
**InchiKey:** GYGSPXRBNGXRQD-LAXRMPOJSA-N  
**Formula:** C31H54  
**SMILES:** CCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3CCCC(C)(C)C3CCC21C  
**Mol. weight [g/mol]:** 426.76

## Physical Properties

Property code	Value	Unit	Source
gf	378.34	kJ/mol	Joback Method
hf	-402.15	kJ/mol	Joback Method
hfus	30.76	kJ/mol	Joback Method
hvap	78.66	kJ/mol	Joback Method
log10ws	-9.61		Crippen Method
logp	9.524		Crippen Method
mcvol	393.350	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	3209.00		NIST Webbook
tb	945.17	K	Joback Method
tc	1181.45	K	Joback Method
tf	567.11	K	Joback Method
vc	1.490	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1528.73	J/mol×K	945.17	Joback Method
cpg	1573.14	J/mol×K	984.55	Joback Method
cpg	1619.88	J/mol×K	1023.93	Joback Method
cpg	1669.59	J/mol×K	1063.31	Joback Method
cpg	1722.91	J/mol×K	1102.69	Joback Method
cpg	1780.46	J/mol×K	1142.07	Joback Method
cpg	1842.88	J/mol×K	1181.45	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=R553609&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R553609&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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