

# 17-«alpha»-H-Homohopane, 22(S)

<b>Inchi:</b>	InChI=1S/C31H54/c1-9-21(2)22-13-18-28(5)23(22)14-19-30(7)25(28)11-12-26-29(6)17-1
<b>InchiKey:</b>	QFBGIDMRCNNMIW-MIOHABFUSA-N
<b>Formula:</b>	C31H54
<b>SMILES:</b>	CCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
<b>Mol. weight [g/mol]:</b>	426.76

## Physical Properties

Property code	Value	Unit	Source
gf	372.85	kJ/mol	Joback Method
hf	-386.91	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-9.61		Crippen Method
logp	9.524		Crippen Method
mvol	393.350	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinpol	3300.00		NIST Webbook
rinpol	3300.00		NIST Webbook
tb	945.41	K	Joback Method
tc	1186.91	K	Joback Method
tf	591.01	K	Joback Method
vc	1.488	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1530.77	J/mol×K	945.41	Joback Method
cpg	1580.09	J/mol×K	985.66	Joback Method
cpg	1633.01	J/mol×K	1025.91	Joback Method
cpg	1690.31	J/mol×K	1066.16	Joback Method
cpg	1752.79	J/mol×K	1106.41	Joback Method
cpg	1821.23	J/mol×K	1146.66	Joback Method
cpg	1896.43	J/mol×K	1186.91	Joback Method

# Sources

<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=R214394&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R214394&amp;Units=SI</a>
<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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