

# Cholesta-4,6-dien-3-ol, (3«beta»)-

<b>Other names:</b>	4,6-Cholestadien-3«beta»-ol cholesta-4,6-diene-3«beta»-ol
<b>Inchi:</b>	InChI=1S/C27H44O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4
<b>InchiKey:</b>	KIULDMFHZZHYKZ-HFRBDLMJSA-N
<b>Formula:</b>	C27H44O
<b>SMILES:</b>	CC(C)CCCC(C)C1CCC2C3C=CC4=CC(O)CCC4(C)C3CCC12C
<b>Mol. weight [g/mol]:</b>	384.64
<b>CAS:</b>	14214-69-8

## Physical Properties

Property code	Value	Unit	Source
gf	233.44	kJ/mol	Joback Method
hf	-429.45	kJ/mol	Joback Method
hfus	37.44	kJ/mol	Joback Method
hvap	90.13	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.165		Crippen Method
mvol	345.120	ml/mol	McGowan Method
pc	1104.47	kPa	Joback Method
tb	946.54	K	Joback Method
tc	1168.01	K	Joback Method
tf	528.15	K	Joback Method
vc	1.308	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.94	J/molxK	946.54	Joback Method
cpg	1315.48	J/molxK	983.45	Joback Method
cpg	1345.55	J/molxK	1020.36	Joback Method
cpg	1376.47	J/molxK	1057.27	Joback Method
cpg	1408.56	J/molxK	1094.18	Joback Method
cpg	1442.14	J/molxK	1131.09	Joback Method
cpg	1477.54	J/molxK	1168.01	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=C14214698&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14214698&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>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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