

# Cholest-5-en-3-ol, (3«alpha»)-

<b>Other names:</b>	Cholest-5-en-3-ol (3 alpha) Epicholesterol
<b>Inchi:</b>	InChI=1S/C27H46O/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>	HVYWMOMLDIMFJA-JKGUEMJCSA-N
<b>Formula:</b>	C27H46O
<b>SMILES:</b>	CC(C)CCCC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
<b>Mol. weight [g/mol]:</b>	386.65
<b>CAS:</b>	474-77-1

## Physical Properties

Property code	Value	Unit	Source
gf	203.48	kJ/mol	Joback Method
hf	-487.23	kJ/mol	Joback Method
hfus	36.22	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.389		Crippen Method
mvol	349.420	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	3055.00		NIST Webbook
tb	947.38	K	Joback Method
tc	1168.23	K	Joback Method
tf	527.39	K	Joback Method
vc	1.321	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1316.89	J/molxK	947.38	Joback Method
cpg	1347.08	J/molxK	984.19	Joback Method
cpg	1377.74	J/molxK	1021.00	Joback Method
cpg	1409.17	J/molxK	1057.80	Joback Method
cpg	1441.71	J/molxK	1094.61	Joback Method
cpg	1475.66	J/molxK	1131.42	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C474771&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C474771&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.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>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>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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