

# Cholestan-3-one, (5«alpha»)-

<b>Other names:</b>	Cholestanone, (5«alpha»)- 5-«alpha»-Cholestan-3-one 5«alpha»-Cholestane-3-one 5«alpha»-Cholestanone 5A-Cholestan-3-one
<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>	PESKGJQREUXSRR-JAGYRSRJSA-N
<b>Formula:</b>	C27H46O
<b>SMILES:</b>	CC(C)CCCC(C)C1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
<b>Mol. weight [g/mol]:</b>	386.65
<b>CAS:</b>	566-88-1

## Physical Properties

Property code	Value	Unit	Source
gf	197.38	kJ/mol	Joback Method
hf	-519.01	kJ/mol	Joback Method
hfus	30.81	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.677		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
tb	918.88	K	Joback Method
tc	1150.52	K	Joback Method
tf	521.51	K	Joback Method
vc	1.323	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.06	J/mol×K	918.88	Joback Method
cpg	1339.92	J/mol×K	957.49	Joback Method
cpg	1371.74	J/mol×K	996.09	Joback Method
cpg	1403.86	J/mol×K	1034.70	Joback Method

cpg	1436.61	J/mol×K	1073.31	Joback Method
cpg	1470.31	J/mol×K	1111.92	Joback Method
cpg	1505.29	J/mol×K	1150.52	Joback Method

## Sources

<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=C566881&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C566881&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>

## 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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