

# 5«alpha»-Cholestan-3«alpha»-ol, 4«alpha»-methyl-, acetate

<b>Other names:</b>	4-Methylcholestan-3-yl acetate, (3«alpha»,4«alpha»,5«alpha»)- 4A-Methylcholestanol acetate
<b>Inchi:</b>	InChI=1S/C30H52O2/c1-19(2)9-8-10-20(3)24-13-14-26-23-11-12-25-21(4)28(32-22(5)31
<b>InchiKey:</b>	WHFNJZOJPBXDDI-FBDHWHPWSA-N
<b>Formula:</b>	C30H52O2
<b>SMILES:</b>	CC(=O)OC1CCC2(C)C(CCC3C4CCC(C(C)CCCC(C)C)C4(C)CCC32)C1C
<b>Mol. weight [g/mol]:</b>	444.73
<b>CAS:</b>	20997-65-3

## Physical Properties

Property code	Value	Unit	Source
gf	95.89	kJ/mol	Joback Method
hf	-728.71	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	87.42	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	8.285		Crippen Method
mcvol	397.560	ml/mol	McGowan Method
pc	832.42	kPa	Joback Method
rinpol	3246.00		NIST Webbook
rinpol	3246.00		NIST Webbook
tb	986.65	K	Joback Method
tc	1214.35	K	Joback Method
tf	550.78	K	Joback Method
vc	1.506	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.59	J/molxK	986.65	Joback Method
cpg	1573.35	J/molxK	1024.60	Joback Method
cpg	1607.39	J/molxK	1062.55	Joback Method
cpg	1642.05	J/molxK	1100.50	Joback Method
cpg	1677.65	J/molxK	1138.45	Joback Method

cpg	1714.51	J/mol×K	1176.40	Joback Method
cpg	1752.96	J/mol×K	1214.35	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=C20997653&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20997653&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>hvac:</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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