

# Cholan-24-oic acid, 3-(acetyloxy)-, methyl ester, (3«alpha»,5«beta»)-

<b>Other names:</b>	5«beta»-Cholanic acid, 3«alpha»-hydroxy-, methyl ester, acetate Acetyllithocholic acid, methyl ester Methyl lithocholate acetate Methyl 3«alpha»-acetoxyolithocholate 3«alpha»-Acetoxy-5«beta»-cholanic acid methyl ester 5«beta»-Cholan-24-oic acid, 3«alpha»-hydroxy-, methyl ester, acetate Methyl 3-O-acetyllithocholate Lithocholic acid, acetate, methyl ester
<b>Inchi:</b>	InChI=1S/C27H44O4/c1-17(6-11-25(29)30-5)22-9-10-23-21-8-7-19-16-20(31-18(2)28)12
<b>InchiKey:</b>	DVIUCIPCTDVQAP-ACCPVXDNSA-N
<b>Formula:</b>	C27H44O4
<b>SMILES:</b>	<chem>COC(=O)CCC(C)C1CCC2C3CCC4CC(OC(C)=O)CCC4(C)C3CCC12C</chem>
<b>Mol. weight [g/mol]:</b>	432.64
<b>CAS:</b>	3253-69-8

## Physical Properties

Property code	Value	Unit	Source
gf	-153.14	kJ/mol	Joback Method
hf	-885.97	kJ/mol	Joback Method
hfus	41.46	kJ/mol	Joback Method
hvap	90.59	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.166		Crippen Method
mcvol	362.730	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	3179.00		NIST Webbook
tb	999.41	K	Joback Method
tc	1232.41	K	Joback Method
tf	608.37	K	Joback Method
vc	1.369	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	1396.53	J/mol×K	999.41	Joback Method
cpg	1427.80	J/mol×K	1038.24	Joback Method
cpg	1459.57	J/mol×K	1077.08	Joback Method
cpg	1492.14	J/mol×K	1115.91	Joback Method
cpg	1525.84	J/mol×K	1154.74	Joback Method
cpg	1560.99	J/mol×K	1193.58	Joback Method
cpg	1597.92	J/mol×K	1232.41	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3253698&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3253698&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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