

# Lithocholic acid

**Other names:**

Cholan-24-oic acid, 3-hydroxy-, (3«alpha»,5«beta»)-  
5«beta»-Cholan-24-oic acid, 3«alpha»-hydroxy-  
Lithocolic acid  
3«alpha»-Hydroxy-5«beta»-cholanic acid  
3«alpha»-Hydroxy-5«beta»-cholanoic acid  
3«alpha»-Hydroxycholanic acid  
3-Hydroxycholan-24-oic acid  
5«beta»-Cholanic acid-3«alpha»-ol  
5-«beta»-Cholanic acid, 3-«alpha»-hydroxy-  
17-«beta»-(1-Methyl-3-carboxypropyl)ethiocholan-3-«alpha»-ol  
NCI-C03861  
3«alpha»-Hydroxy-5«beta»-cholan-24-oic acid  
NSC 683770

**Inchi:**

InChI=1S/C24H40O3/c1-15(4-9-22(26)27)19-7-8-20-18-6-5-16-14-17(25)10-12-23(16,2)24

**InchiKey:**

SMEROWZSTRWXGI-VKPXTEDRSA-N

**Formula:**

C24H40O3

**SMILES:**

CC(CCC(=O)O)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C

**Mol. weight [g/mol]:**

376.57

**CAS:**

434-13-9

## Physical Properties

Property code	Value	Unit	Source
gf	-113.12	kJ/mol	Joback Method
hf	-751.49	kJ/mol	Joback Method
hfus	37.90	kJ/mol	Joback Method
hvap	105.71	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.507		Crippen Method
mcvol	318.890	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
tb	1016.42	K	Joback Method
tc	1245.60	K	Joback Method
tf	462.00 ± 4.00	K	NIST Webbook
vc	1.198	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1266.26	J/mol×K	1016.42	Joback Method
cpg	1296.46	J/mol×K	1054.62	Joback Method
cpg	1327.80	J/mol×K	1092.81	Joback Method
cpg	1360.63	J/mol×K	1131.01	Joback Method
cpg	1395.29	J/mol×K	1169.20	Joback Method
cpg	1432.10	J/mol×K	1207.40	Joback Method
cpg	1471.43	J/mol×K	1245.60	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=C434139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C434139&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>

## 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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