

# Cholesteryl chloroacetate

<b>Other names:</b>	Cholest-5-en-3-ol (3«beta»)-, chloroacetate 3Beta-chloroacetoxycholest-5-ene 3«beta»-(Chloroacetoxo)cholest-5-ene cholest-5-ene-3-«beta»-yl chloroacetate
<b>Inchi:</b>	InChI=1S/C29H47ClO2/c1-19(2)7-6-8-20(3)24-11-12-25-23-10-9-21-17-22(32-27(31)18-
<b>InchiKey:</b>	XUXXPLDKUZSGKH-FOBBRWMUSA-N
<b>Formula:</b>	C29H47ClO2
<b>SMILES:</b>	<chem>CC(C)CCCC(C)C1CCC2C3CC=C4CC(OC(=O)CCl)CCC4(C)C3CCC12C</chem>
<b>Mol. weight [g/mol]:</b>	463.13
<b>CAS:</b>	3464-50-4

## Physical Properties

Property code	Value	Unit	Source
gf	111.29	kJ/mol	Joback Method
hf	-636.82	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	91.15	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	8.178		Crippen Method
mcvol	391.410	ml/mol	McGowan Method
pc	907.24	kPa	Joback Method
tb	1014.68	K	Joback Method
tc	1248.99	K	Joback Method
tf	591.19	K	Joback Method
vc	1.488	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1472.87	J/molxK	1014.68	Joback Method
cpg	1506.26	J/molxK	1053.73	Joback Method
cpg	1540.55	J/molxK	1092.78	Joback Method
cpg	1576.10	J/molxK	1131.84	Joback Method
cpg	1613.28	J/molxK	1170.89	Joback Method

cpg	1652.44	J/mol×K	1209.94	Joback Method
cpg	1693.96	J/mol×K	1248.99	Joback Method

## Sources

<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=C3464504&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3464504&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>

## 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>hvp:</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>mcpol:</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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