

# 22-Dehydrocholesterol (Z) acetate

<b>Inchi:</b>	InChI=1S/C29H46O2/c1-19(2)8-7-9-20(3)25-12-13-26-24-11-10-22-18-23(31-21(4)30)14
<b>InchiKey:</b>	CJUZRUVXJPNXNH-ROGDJRGZSA-N
<b>Formula:</b>	C29H46O2
<b>SMILES:</b>	CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)C=CCC(C)C)CCC32)C1
<b>Mol. weight [g/mol]:</b>	426.67

## Physical Properties

Property code	Value	Unit	Source
gf	203.44	kJ/mol	Joback Method
hf	-503.86	kJ/mol	Joback Method
hfus	40.30	kJ/mol	Joback Method
hvap	86.72	kJ/mol	Joback Method
log10ws	-8.29		Crippen Method
logp	7.736		Crippen Method
mvol	374.870	ml/mol	McGowan Method
pc	957.91	kPa	Joback Method
rinpol	3134.00		NIST Webbook
rinpol	3134.00		NIST Webbook
tb	981.41	K	Joback Method
tc	1214.58	K	Joback Method
tf	556.19	K	Joback Method
vc	1.419	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1405.99	J/molxK	981.41	Joback Method
cpg	1438.81	J/molxK	1020.27	Joback Method
cpg	1472.37	J/molxK	1059.13	Joback Method
cpg	1507.05	J/molxK	1097.99	Joback Method
cpg	1543.22	J/molxK	1136.85	Joback Method
cpg	1581.24	J/molxK	1175.72	Joback Method
cpg	1621.50	J/molxK	1214.58	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R110059&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R110059&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>
<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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</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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