

# 3Beta-hydroxy-24beta-methyl-5alpha-cholest-14-en-20-one benzoate

InChI:	InChI=1S/C35H52O2/c1-23(2)24(3)12-13-25(4)30-16-17-31-29-15-14-27-22-28(37-33(36)35)21
InChIKey:	PXRZGKIPOGDNPV-UHFFFAOYSA-N
Formula:	C35H52O2
SMILES:	CC(C)C(C)CCC(C)C1CC=C2C3CCC4CC(OC(=O)c5ccccc5)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	504.79
CAS:	6034-20-4

## Physical Properties

Property code	Value	Unit	Source
gf	283.71	kJ/mol	Joback Method
hf	-513.67	kJ/mol	Joback Method
hfus	46.15	kJ/mol	Joback Method
hvap	102.01	kJ/mol	Joback Method
log10ws	-10.39		Crippen Method
logp	9.499		Crippen Method
mcvol	439.950	ml/mol	McGowan Method
pc	807.08	kPa	Joback Method
tb	1140.77	K	Joback Method
tc	1398.05	K	Joback Method
tf	640.31	K	Joback Method
vc	1.661	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1776.51	J/molxK	1140.77	Joback Method
cpg	1820.18	J/molxK	1183.65	Joback Method
cpg	1866.28	J/molxK	1226.53	Joback Method
cpg	1915.33	J/molxK	1269.41	Joback Method
cpg	1967.85	J/molxK	1312.29	Joback Method
cpg	2024.37	J/molxK	1355.17	Joback Method
cpg	2085.41	J/molxK	1398.05	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6034204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6034204&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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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