Cholest-5-en-3-ol (3«beta»)-, acetate

Other names:	Cholesterol, acetate
	(-)-Cholesteryl acetate
	Cholest-5-en-3«beta»-ol acetate
	Cholest-5-en-3«beta»-yl acetate
	Cholesterin acetate
	Cholesteryl acetate
	3«beta»-Acetoxycholest-5-ene
	5-Cholesten-3«beta»-ol acetate
	Cholest-5-en-3-yl acetate, (3«beta»)-
	5-Cholesten-3-beta-ol, acetate
	3-Cholesteryl acetate
	NSC 8799
	5-Cholesten-3B-ol, acetate
Inchi:	InChI=1S/C29H48O2/c1-19(2)8-7-9-20(3)25-12-13-26-24-11-10-22-18-23(31-21(4)30)14
InchiKey:	XUGISPSHIFXEHZ-WOOIZHOCSA-N
Formula:	C29H48O2
SMILES:	CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]:	428.69
CAS:	604-35-3

Physical Properties

Property code	Value	Unit	Source
gf	123.22	kJ/mol	Joback Method
hf	-621.08	kJ/mol	Joback Method
hfus	40.10	kJ/mol	Joback Method
hvap	86.76	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	7.960		Crippen Method
mcvol	379.170	ml/mol	McGowan Method
pc	927.81	kPa	Joback Method
rinpol	3182.00		NIST Webbook
rinpol	3135.00		NIST Webbook
tb	977.25	K	Joback Method
tc	1206.29	K	Joback Method
tf	387.80 ± 0.50	K	NIST Webbook
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.94	J/mol×K	977.25	Joback Method
cpg	1465.33	J/mol×K	1015.42	Joback Method
cpg	1498.23	J/mol×K	1053.60	Joback Method
cpg	1531.96	J/mol×K	1091.77	Joback Method
cpg	1566.85	J/mol×K	1129.94	Joback Method
cpg	1603.25	J/mol×K	1168.11	Joback Method
cpg	1641.50	J/mol×K	1206.29	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C604353&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume