Cholesta-5,7-dien-3-ol, acetate, (3«beta»)-

Other names:	Cholesta-5,7-dien-3«beta»-ol, acetate
	Cholest-5,7-dien-3«beta»-yl acetate
	Cholesta-5,7-dien-3«beta»-yl acetate
	3«beta»-Acetoxychoesta-5,7-diene
	7-Dehydrocholesterol acetate
	7-Dehydrocholesteryl acetate
	Cholesta-5,7-dien-3-yl acetate, (3«beta»)-
	7,8-Didehydrocholesterol acetate
	NSC 226869
Inchi:	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
InchiKey:	ACGNVBRAISEVDK-AYYXOLOQSA-N
Formula:	C29H46O2
SMILES:	CC(=O)OC1CCC2(C)C(=CC=C3C2CCC2(C)C3CCC2C(C)CCCC(C)C)C1
Mol. weight [g/mol]:	426.67
CAS:	1059-86-5

Physical Properties

Property code	Value	Unit	Source
gf	151.26	kJ/mol	Joback Method
hf	-554.43	kJ/mol	Joback Method
hfus	39.86	kJ/mol	Joback Method
hvap	88.03	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.880		Crippen Method
mcvol	374.870	ml/mol	McGowan Method
pc	959.10	kPa	Joback Method
tb	986.06	K	Joback Method
tc	1217.09	K	Joback Method
tf	578.79	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1399.64	J/mol×K	986.06	Joback Method
cpg	1431.74	J/mol×K	1024.56	Joback Method
cpg	1464.57	J/mol×K	1063.07	Joback Method
cpg	1498.48	J/mol×K	1101.57	Joback Method
cpg	1533.81	J/mol×K	1140.08	Joback Method
cpg	1570.91	J/mol×K	1178.58	Joback Method
cpg	1610.13	J/mol×K	1217.09	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1059865&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume