Cholesta-8,24-dien-3-ol, acetate, (3«beta»,5«alpha»)-

Other names: 5«alpha»-Cholesta-8,24-dien-3«beta»-ol, acetate
Zymosterol acetate
Cholesta-8,24-dien-3-yl acetate, (3«beta»,5«alpha»)-

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: ICNJVDYAAWEPCH-GPDNFOSISA-N

Formula: C29H46O2

SMILES: CC(=O)OC1CCC2(C)C3=C(CCC2C1)C1CCC(C(C)CCC=C(C)C)C1(C)CC3

Mol. weight [g/mol]: 426.67

CAS: 2579-07-9

Physical Properties

Property code	Value	Unit	Source
gf	195.41	kJ/mol	Joback Method
hf	-499.50	kJ/mol	Joback Method
hfus	41.05	kJ/mol	Joback Method
hvap	88.16	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	8.024		Crippen Method
mcvol	374.870	ml/mol	McGowan Method
pc	966.87	kPa	Joback Method
rinpol	3237.00		NIST Webbook
tb	991.38	K	Joback Method
tc	1225.48	K	Joback Method
tf	573.99	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1403.83	J/mol×K	991.38	Joback Method
cpg	1437.07	J/mol×K	1030.40	Joback Method
cpg	1471.26	J/mol×K	1069.41	Joback Method
cpg	1506.76	J/mol×K	1108.43	Joback Method
cpg	1543.95	J/mol×K	1147.45	Joback Method

cpg	1583.22	J/mol×K	1186.46	Joback Method
cpg	1624.94	J/mol×K	1225.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2579079&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

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