5A-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-CEEZXXFPSA-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

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	3142.00		NIST Webbook
tb	977.25	K	Joback Method
tc	1206.29	K	Joback Method
tf	561.27	K	Joback Method
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

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=R91418&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume