22-Dehydrocholesterol (E) acetate

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: CJUZRVVXJPNXNH-XVVDPDAXSA-N
Formula: C29H46O2
SMILES: CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)C=CCC(C)C)CCC32)C1
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	203.44	kJ/mol	Joback Method
hf	-503.86	kJ/mol	Joback Method
hfus	40.30	kJ/mol	Joback Method
hvap	86.72	kJ/mol	Joback Method
log10ws	-8.29		Crippen Method
logp	7.736		Crippen Method
mcvol	374.870	ml/mol	McGowan Method
pc	957.91	kPa	Joback Method
rinpol	3151.00		NIST Webbook
tb	981.41	K	Joback Method
tc	1214.58	K	Joback Method
tf	556.19	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1405.99	J/mol×K	981.41	Joback Method
cpg	1438.81	J/mol×K	1020.27	Joback Method
cpg	1472.37	J/mol×K	1059.13	Joback Method
cpg	1507.05	J/mol×K	1097.99	Joback Method
cpg	1543.22	J/mol×K	1136.85	Joback Method
cpg	1581.24	J/mol×K	1175.72	Joback Method
cpg	1621.50	J/mol×K	1214.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110044&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