24-Methylenecholesterol acetate

Inchi: InChI=1S/C30H48O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31)
InchiKey: ZWFFFDGHCKZGQM-BTDHWFDRSA-N
Formula: C30H48O2
SMILES: C=C(CCC(C)C1CCC2C3CCC4=CC(OC(C)=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	210.93	kJ/mol	Joback Method
hf	-526.08	kJ/mol	Joback Method
hfus	40.10	kJ/mol	Joback Method
hvap	88.40	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.126		Crippen Method
mcvol	388.960	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	3272.00		NIST Webbook
tb	996.69	K	Joback Method
tc	1229.29	K	Joback Method
tf	556.82	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1472.17	J/mol×K	996.69	Joback Method
cpg	1505.66	J/mol×K	1035.46	Joback Method
cpg	1539.89	J/mol×K	1074.22	Joback Method
cpg	1575.24	J/mol×K	1112.99	Joback Method
cpg	1612.05	J/mol×K	1151.76	Joback Method
cpg	1650.70	J/mol×K	1190.52	Joback Method
cpg	1691.54	J/mol×K	1229.29	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=R87455&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