4A-Methyl-8-cholestenol acetate

Inchi: InChI=1S/C30H50O2/c1-19(2)9-8-10-20(3)24-13-14-26-23-11-12-25-21(4)28(32-22(5)31)
InchiKey: HTILMTUGTYOTQK-ZDQOXHSUSA-N
Formula: C30H50O2
SMILES: CC(=O)OC1CCC2(C)C3=C(CCC2C1C)C1CCC(C(C)CCCC(C)C)C1(C)CC3
Mol. weight [g/mol]: 442.72

Physical Properties

Property code	Value	Unit	Source
gf	122.01	kJ/mol	Joback Method
hf	-653.19	kJ/mol	Joback Method
hfus	42.30	kJ/mol	Joback Method
hvap	89.65	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	8.350		Crippen Method
mcvol	393.260	ml/mol	McGowan Method
pc	868.11	kPa	Joback Method
rinpol	3253.00		NIST Webbook
rinpol	3253.00		NIST Webbook
tb	1005.11	K	Joback Method
tc	1236.26	K	Joback Method
tf	585.06	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1505.21	J/mol×K	1005.11	Joback Method
cpg	1539.03	J/mol×K	1043.64	Joback Method
cpg	1573.53	J/mol×K	1082.16	Joback Method
cpg	1609.04	J/mol×K	1120.69	Joback Method
cpg	1645.91	J/mol×K	1159.21	Joback Method
cpg	1684.48	J/mol×K	1197.74	Joback Method
cpg	1725.10	J/mol×K	1236.26	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=R110737&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