4,4-Dimethylcholestanol acetate

Inchi: InChI=1S/C31H54O2/c1-20(2)10-9-11-21(3)24-13-14-25-23-12-15-27-29(5,6)28(33-22(4)
InchiKey: NRAWTYCKLCALTN-MGWJKQGHSA-N
Formula: C31H54O2
SMILES: CC(=O)OC1CCC2(C)C3CCC4(C)C(C(C)CCCC(C)C)CCC4C3CCC2C1(C)C
Mol. weight [g/mol]: 458.76

Physical Properties

Property code	Value	Unit	Source
gf	98.82	kJ/mol	Joback Method
hf	-734.11	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	88.49	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	8.675		Crippen Method
mcvol	411.650	ml/mol	McGowan Method
pc	808.45	kPa	Joback Method
rinpol	3316.00		NIST Webbook
tb	1009.77	K	Joback Method
tc	1241.64	K	Joback Method
tf	585.95	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1620.48	J/mol×K	1009.77	Joback Method
cpg	1661.32	J/mol×K	1048.42	Joback Method
cpg	1703.82	J/mol×K	1087.06	Joback Method
cpg	1748.45	J/mol×K	1125.71	Joback Method
cpg	1795.64	J/mol×K	1164.35	Joback Method
cpg	1845.85	J/mol×K	1203.00	Joback Method
cpg	1899.52	J/mol×K	1241.64	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=R110693&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

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