D7-Campesterol acetate

Other names: 5,7-Ergostadienol 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: OEQXNFVIQLJFHG-NQNNFHKGSA-N
Formula: C30H48O2
SMILES: CC(=O)OC1CCC2(C)C(=CC=C3C2CCC2(C)C3CCC2C(C)CCC(C)C(C)C)C1
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	157.24	kJ/mol	Joback Method
hf	-580.35	kJ/mol	Joback Method
hfus	38.93	kJ/mol	Joback Method
hvap	89.87	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.126		Crippen Method
mcvol	388.960	ml/mol	McGowan Method
pc	908.89	kPa	Joback Method
rinpol	3323.00		NIST Webbook
tb	1008.50	K	Joback Method
tc	1242.10	K	Joback Method
tf	575.06	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1470.58	J/mol×K	1008.50	Joback Method
cpg	1504.16	J/mol×K	1047.43	Joback Method
cpg	1538.62	J/mol×K	1086.37	Joback Method
cpg	1574.34	J/mol×K	1125.30	Joback Method
cpg	1611.67	J/mol×K	1164.23	Joback Method
cpg	1650.98	J/mol×K	1203.16	Joback Method
cpg	1692.64	J/mol×K	1242.10	Joback Method

Sources

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=R87530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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