Ergosta-7,22-dien-3-ol, acetate, (3«beta»,5«alpha»)-

Other names: Ergosta-7,22-dien-3«beta»-ol, acetate
5«alpha»-Ergost-7,22-dien-3«beta»-ol acetate
7,22-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: MXEWOTISHNVRHW-OVHCQGATSA-N

Formula: C30H48O2

SMILES: CC(=O)OC1CCC2(C)C(CC=C3C2CCC2(C)C3CCC2C(C)C=CC(C)C(C)C)C1

Mol. weight [g/mol]: 440.70

CAS: 1449-60-1

Physical Properties

Property code	Value	Unit	Source
gf	209.42	kJ/mol	Joback Method
hf	-529.78	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	88.56	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.982		Crippen Method
mcvol	388.960	ml/mol	McGowan Method
pc	907.79	kPa	Joback Method
rinpol	3269.00		NIST Webbook
rinpol	3269.00		NIST Webbook
tb	1003.85	K	Joback Method
tc	1239.22	K	Joback Method
tf	552.46	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1477.08	J/mol×K	1003.85	Joback Method
cpg	1511.34	J/mol×K	1043.08	Joback Method
cpg	1546.51	J/mol×K	1082.31	Joback Method
cpg	1582.99	J/mol×K	1121.54	Joback Method

cpg	1621.14	J/mol×K	1160.76	Joback Method
cpg	1661.37	J/mol×K	1199.99	Joback Method
cpg	1704.06	J/mol×K	1239.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1449601&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