

Ergosta-5,7,22-trien-3-ol, acetate, (3«beta»,22E)-

Other names:	Ergosterol, acetate Ergosta-5,7,22-trien-3«beta»-yl acetate Ergosteryl acetate Ergosteryl 3«beta»-acetate Ergosterin acetate Ergosta-5,7,22-trien-3«beta»-ol, acetate (3«beta»,22E)-Ergosta-5,7,22-trien-3-yl acetate
Inchi:	InChI=1S/C30H46O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31
InchiKey:	NGEVNHYPVVOXPB-FFVIOIHDSA-N
Formula:	C30H46O2
SMILES:	CC(=O)OC1CCC2(C)C(=CC=C3C2CCC2(C)C3CCC2C(C)C=CC(C)C(C)C)C1
Mol. weight [g/mol]:	438.69
CAS:	2418-45-3

Physical Properties

Property code	Value	Unit	Source
gf	237.46	kJ/mol	Joback Method
hf	-463.13	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	89.82	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.902		Crippen Method
mvol	384.660	ml/mol	McGowan Method
pc	938.07	kPa	Joback Method
rinpol	3269.00		NIST Webbook
tb	1012.66	K	Joback Method
tc	1250.02	K	Joback Method
tf	569.98	K	Joback Method
vc	1.456	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1443.50	J/mol×K	1012.66	Joback Method

cpg	1477.64	J/mol×K	1052.22	Joback Method
cpg	1512.96	J/mol×K	1091.78	Joback Method
cpg	1549.84	J/mol×K	1131.34	Joback Method
cpg	1588.69	J/mol×K	1170.90	Joback Method
cpg	1629.91	J/mol×K	1210.46	Joback Method
cpg	1673.90	J/mol×K	1250.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2418453&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

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