Ergosta-7,24(28)-dien-3-ol, 4-methyl-, acetate, (3«beta»,4«alpha»)-

Other names: 4-Methylergosta-7,24(28)-dien-3-yl acetate, (3«beta»,4«alpha»)-
24-Methyl-24(25)-dehydrolophenol acetate
Gramisterol (24-methylenelophenol) acetate

Inchi: InChI=1S/C31H50O2/c1-19(2)20(3)9-10-21(4)25-13-14-27-24-11-12-26-22(5)29(33-23(6

InchiKey: ATSVMNCIUVPBNE-UHFFFAOYSA-N

Formula: C31H50O2

SMILES: C=C(CCC(C)C1CCC2C3=CCC4C(C)C(OC(C)=O)CCC4(C)C3CCC21C)C(C)C

Mol. weight [g/mol]: 454.73

CAS: 55399-28-5

Physical Properties

Property code	Value	Unit	Source
gf	211.64	kJ/mol	Joback Method
hf	-567.06	kJ/mol	Joback Method
hfus	43.76	kJ/mol	Joback Method
hvap	90.32	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	8.372		Crippen Method
mcvol	403.050	ml/mol	McGowan Method
pc	834.83	kPa	Joback Method
rinpol	3364.00		NIST Webbook
rinpol	3416.00		NIST Webbook
tb	1014.90	K	Joback Method
tc	1248.26	K	Joback Method
tf	563.85	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1546.39	J/mol×K	1014.90	Joback Method
cpg	1581.01	J/mol×K	1053.79	Joback Method
cpg	1616.40	J/mol×K	1092.69	Joback Method
cpg	1652.91	J/mol×K	1131.58	Joback Method

cpg	1690.92	J/mol×K	1170.48	Joback Method
cpg	1730.79	J/mol×K	1209.37	Joback Method
cpg	1772.86	J/mol×K	1248.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55399285&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