

Ergosta-5,24-dien-3-ol, acetate, (3«beta»)-

Other names:	Ergosta-5,24-dien-3«beta»-ol, acetate 24-Methylcholesta-5,24-dien-3«beta»-yl acetate Ergosta-5,24-dien-3-yl acetate, (3«beta»)- 5,24-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:	LUSJRANTKUMKJQ-XGIAZTPUSA-N
Formula:	C30H48O2
SMILES:	CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCC(C)=C(C)C)CCC32)C1
Mol. weight [g/mol]:	440.70
CAS:	33444-85-8

Physical Properties

Property code	Value	Unit	Source
gf	197.20	kJ/mol	Joback Method
hf	-538.80	kJ/mol	Joback Method
hfus	43.79	kJ/mol	Joback Method
hvap	89.50	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.270		Crippen Method
mcvol	388.960	ml/mol	McGowan Method
pc	904.52	kPa	Joback Method
rinpol	3323.00		NIST Webbook
rinpol	3323.00		NIST Webbook
tb	1004.49	K	Joback Method
tc	1239.37	K	Joback Method
tf	554.54	K	Joback Method
vc	1.482	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1476.04	J/mol×K	1004.49	Joback Method
cpg	1510.48	J/mol×K	1043.64	Joback Method
cpg	1545.88	J/mol×K	1082.78	Joback Method

cpg	1582.64	J/mol×K	1121.93	Joback Method
cpg	1621.13	J/mol×K	1161.07	Joback Method
cpg	1661.74	J/mol×K	1200.22	Joback Method
cpg	1704.86	J/mol×K	1239.37	Joback Method

Sources

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=C33444858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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