

Lanosta-7,9(11)-dien-3-ol, acetate, (3«beta»)-

Other names:	Lanosta-7,9(11)-dien-3«beta»-ol, acetate Dihydroagnosterol acetate 3«beta»-Acetoxylanosta-7,9(11)-diene Lanosta-7,9(11)-dien-3-yl acetate, (3«beta»)- 24-Dihydroagnosterol acetate
Inchi:	InChI=1S/C32H52O2/c1-21(2)11-10-12-22(3)24-15-19-32(9)26-13-14-27-29(5,6)28(34-2
InchiKey:	FGNFBQUIVUFRIF-MTJKDGKCSA-N
Formula:	C32H52O2
SMILES:	CC(=O)OC1CCC2(C)C3=CCC4(C)C(C(C)CCCC(C)C)CCC4(C)C3=CCC2C1(C)C
Mol. weight [g/mol]:	468.75
CAS:	5600-01-1

Physical Properties

Property code	Value	Unit	Source
gf	157.83	kJ/mol	Joback Method
hf	-606.21	kJ/mol	Joback Method
hfus	36.10	kJ/mol	Joback Method
hvap	92.09	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.906		Crippen Method
mcvol	417.140	ml/mol	McGowan Method
pc	835.31	kPa	Joback Method
rinpol	3286.00		NIST Webbook
rinpol	3286.00		NIST Webbook
tb	1050.51	K	Joback Method
tc	1290.54	K	Joback Method
tf	656.16	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1647.06	J/mol×K	1050.51	Joback Method
cpg	1698.15	J/mol×K	1090.52	Joback Method

cpg	1753.23	J/mol×K	1130.52	Joback Method
cpg	1812.93	J/mol×K	1170.53	Joback Method
cpg	1877.86	J/mol×K	1210.53	Joback Method
cpg	1948.66	J/mol×K	1250.54	Joback Method
cpg	2025.93	J/mol×K	1290.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5600011&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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