

Ergosta-5,7,22-trien-3-ol, acetate, (3.β.,22e)-

Other names:	Ergosterol, acetate Ergosta-5,7,22-trien-3«β»-yl acetate Ergosteryl acetate Ergosteryl 3«β»-acetate Ergosterin acetate Ergosta-5,7,22-trien-3«β»-ol, acetate (3«β»,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)O[C@H]1CCC2(C)C(=CC=C3C2CCC2(C)C3CCC2C(C)/C=C/C(C)C(C)C)C1
Mol. weight [g/mol]:	438.70

Physical Properties

Property code	Value	Unit	Source
hfus	39.13	kJ/mol	Joback Method
logp	7.902		Crippen Method
mcvol	384.660	ml/mol	McGowan Method
rinpol	3269.00		NIST Webbook
tf	422.69	K	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2418453&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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