

9,19-Cycloergost-24(28)-en-3-ol, 4,14-dimethyl-, acetate, (3«beta»,4«alpha»,5«alpha»)-

Other names

Cycloergostenyl acetate
Cycloergostenol acetate

Inchi:	9,19-Cyclo-5«alpha»,9«beta»-ergost-24(28)-en-3«beta»-ol, 4«alpha»,14-dimethyl-, acetate
InchiKey:	QEBAXZCXAFWBDK-UHFFFAOYSA-N
Formula:	C32H52O2
SMILES:	C=C(CCC(C)C1CCC2(C)C3CCC4C(C)C(OC(C)=O)CCC45CC3CCC12C)C(C)C
Mol. weight [g/mol]:	468.75
CAS:	10376-42-8

Physical Properties

Property code	Value	Unit	Source
gf	273.70	kJ/mol	Joback Method
hf	-518.41	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	88.86	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	861.00	kPa	Joback Method
rinpol	3378.00		NIST Webbook
rinpol	3378.00		NIST Webbook
tb	1032.32	K	Joback Method
tc	1270.96	K	Joback Method
tf	634.62	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1649.30	J/molxK	1032.32	Joback Method
cpg	1700.86	J/molxK	1072.09	Joback Method
cpg	1756.63	J/molxK	1111.87	Joback Method
cpg	1817.30	J/molxK	1151.64	Joback Method

cpg	1883.55	J/mol×K	1191.41	Joback Method
cpg	1956.06	J/mol×K	1231.19	Joback Method
cpg	2035.52	J/mol×K	1270.96	Joback Method

Sources

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=C10376428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mvol:	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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