3-O-Acetyl-Delta24-Cycloartenol

Other names: Cycloeucalenyl acetate
Cycloeucalenol acetate
9,19-Cyclo-5«alpha»,9«beta»-ergost-24(28)-en-3«beta»-ol, 4«alpha»,14-dimethyl-, acetate
Inchi: InChI=1S/C32H52O2/c1-20(2)21(3)9-10-22(4)25-13-15-30(8)28-12-11-26-23(5)27(34-24
InchiKey: QEBAXZCXAFWBDK-UHFFFAOYSA-N
Formula: C32H52O2
SMILES: C=C(CCC(C)C1CCC2(C)C3CCC4C(C)C(OC(C)=O)CCC45CC35CCC12C)C(C)C
Mol. weight [g/mol]: 468.77

Physical Properties

Property code	Value	Unit	Source
hfus	35.25	kJ/mol	Joback Method
logp	8.596		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
rinpol	3378.00		NIST Webbook
rinpol	3378.00		NIST Webbook

Temperature Dependent Properties

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

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=C10376428&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