

9,19-Cyclolanost-24-en-3-ol, acetate, (3«beta»)-

Other names:

9,19-Cyclo-9«beta»-lanost-24-en-3«beta»-ol, acetate

Cycloartenol acetate

Cycloartenyl acetate

3-O-Acetylcycloartenol

1H,19H-Cyclopropa[9,10]cyclopenta[a]phenanthrene, 9,19-cyclolanost-24-en-3-ol deriv
Cycloartenol 3-acetate

Inchi: InChI=1S/C32H52O2/c1-21(2)10-9-11-22(3)24-14-16-30(8)26-13-12-25-28(5,6)27(34-23

InchiKey: PQNTWKDHNSWVPU-UHFFFAOYSA-N

Formula: C32H52O2

SMILES: CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CCC=C(C)C)CCC2(C)C4CCC3C1(C)C

Mol. weight [g/mol]: 468.75

CAS: 1259-10-5

Physical Properties

Property code	Value	Unit	Source
gf	263.03	kJ/mol	Joback Method
hf	-506.10	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.740		Crippen Method
mvol	410.580	ml/mol	McGowan Method
pc	885.24	kPa	Joback Method
rinpol	3389.00		NIST Webbook
rinpol	3389.00		NIST Webbook
tb	1040.48	K	Joback Method
tc	1282.98	K	Joback Method
tf	670.20	K	Joback Method
vc	1.573	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.25	J/mol×K	1040.48	Joback Method

cpg	1730.89	J/mol×K	1080.90	Joback Method
cpg	1797.58	J/mol×K	1121.31	Joback Method
cpg	1871.17	J/mol×K	1161.73	Joback Method
cpg	1952.53	J/mol×K	1202.15	Joback Method
cpg	2042.48	J/mol×K	1242.57	Joback Method
cpg	2141.88	J/mol×K	1282.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C1259105&Units=SI

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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