3-O-Acetyl-Cycloartenol

Other names:	1H,19H-Cyclopropa[9,10]cyclopenta[a]phenanthrene, 9,19-cyclolanost-24-en-3-ol deriv.
	3-O-Acetylcycloartenol
	9,19-Cyclo-9«beta»-lanost-24-en-3«beta»-ol, acetate
	Cycloartenol 3-acetate
	Cycloartenol acetate
	Cycloartenyl 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]:	468.77

Physical Properties

Property code	Value	Unit	Source
hfus	33.96	kJ/mol	Joback Method
logp	8.740		Crippen Method
mcvol	410.580	ml/mol	McGowan 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:	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=C1259105&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