9,19-CYCLO-9.BETA.-LANOST-7-EN-3.BETA.-OL, ACETATE

Other names: 24-Dihydrocimicifugenol 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: QXHRYQRNDMKNRQ-UHFFFAOYSA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CCCC(C)C)CCC2(C)C4=CCC3C1(C)C
Mol. weight [g/mol]: 468.77

Physical Properties

Property code	Value	Unit	Source
hfus	31.31	kJ/mol	Joback Method
logp	8.740		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
rinpol	3256.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1666.16	J/mol×K	1044.81	Joback Method
cpg	1726.28	J/mol×K	1084.98	Joback Method
cpg	1792.38	J/mol×K	1125.16	Joback Method
cpg	1865.27	J/mol×K	1165.33	Joback Method
cpg	1945.77	J/mol×K	1205.51	Joback Method
cpg	2034.68	J/mol×K	1245.68	Joback Method
cpg	2132.83	J/mol×K	1285.85	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C28413798&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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