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]: 468.75
CAS: 28413-79-8

Physical Properties

Property code	Value	Unit	Source
gf	216.96	kJ/mol	Joback Method
hf	-552.16	kJ/mol	Joback Method
hfus	31.31	kJ/mol	Joback Method
hvap	89.56	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.740		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	887.88	kPa	Joback Method
rinpol	3256.00		NIST Webbook
rinpol	3256.00		NIST Webbook
tb	1044.81	K	Joback Method
tc	1285.85	K	Joback Method
tf	691.76	K	Joback Method
vc	1.573	m3/kmol	Joback Method

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:	https://www.chemeo.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=C28413798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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