24-Ethyl-31-nor-8-lanostenol acetate

Inchi: InChI=1S/C33H56O2/c1-10-24(11-2)13-12-22(3)25-16-20-33(9)27-14-15-28-30(5,6)29(3
InchiKey: DRCQEZRGSGKPFW-XPPNMVHISA-N
Formula: C33H56O2
SMILES: CCC(CC)CCC(C)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(OC(C)=O)C(C)(C)C1CC3
Mol. weight [g/mol]: 484.80

Physical Properties

Property code	Value	Unit	Source
gf	136.29	kJ/mol	Joback Method
hf	-684.63	kJ/mol	Joback Method
hfus	37.47	kJ/mol	Joback Method
hvap	94.03	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	9.520		Crippen Method
mcvol	435.530	ml/mol	McGowan Method
pc	775.05	kPa	Joback Method
rinpol	3414.00		NIST Webbook
tb	1074.23	K	Joback Method
tc	1316.65	K	Joback Method
tf	666.67	K	Joback Method
vc	1.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1762.51	J/mol×K	1074.23	Joback Method
cpg	1817.73	J/mol×K	1114.63	Joback Method
cpg	1877.27	J/mol×K	1155.04	Joback Method
cpg	1941.77	J/mol×K	1195.44	Joback Method
cpg	2011.88	J/mol×K	1235.84	Joback Method
cpg	2088.24	J/mol×K	1276.25	Joback Method
cpg	2171.50	J/mol×K	1316.65	Joback Method

Sources

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=R110331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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