31-Nor-8-lanostenol acetate

Inchi: InChI=1S/C31H52O2/c1-9-10-11-12-21(2)23-15-19-31(8)25-13-14-26-28(4,5)27(33-22(3)
InchiKey: ZBDUOBKAXCMJNN-IDVHDOOBSA-N
Formula: C31H52O2
SMILES: CCCCCC(C)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(OC(C)=O)C(C)(C)C1CC3
Mol. weight [g/mol]: 456.74

Physical Properties

Property code	Value	Unit	Source
gf	121.89	kJ/mol	Joback Method
hf	-638.07	kJ/mol	Joback Method
hfus	35.81	kJ/mol	Joback Method
hvap	89.96	kJ/mol	Joback Method
log10ws	-9.51		Crippen Method
logp	8.884		Crippen Method
mcvol	407.350	ml/mol	McGowan Method
pc	861.00	kPa	Joback Method
rinpol	3243.00		NIST Webbook
rinpol	3243.00		NIST Webbook
tb	1028.91	K	Joback Method
tc	1265.42	K	Joback Method
tf	659.13	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1600.03	J/mol×K	1028.91	Joback Method
cpg	1648.38	J/mol×K	1068.33	Joback Method
cpg	1700.27	J/mol×K	1107.75	Joback Method
cpg	1756.26	J/mol×K	1147.17	Joback Method
cpg	1816.97	J/mol×K	1186.58	Joback Method
cpg	1882.96	J/mol×K	1226.00	Joback Method
cpg	1954.84	J/mol×K	1265.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R110633&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