4A-Methyl-8(14)-ergostenol acetate

Inchi: InChI=1S/C31H52O2/c1-19(2)20(3)9-10-21(4)25-13-14-27-24-11-12-26-22(5)29(33-23(6)
InchiKey: MECHFHDTOVPIKF-VOEFFRNLSA-N
Formula: C31H52O2
SMILES: CC(=O)OC1CCC2(C)C3CCC4(C)C(=C3CCC2C1C)CCC4C(C)CCC(C)C(C)C
Mol. weight [g/mol]: 456.74

Physical Properties

Property code	Value	Unit	Source
gf	127.99	kJ/mol	Joback Method
hf	-679.11	kJ/mol	Joback Method
hfus	41.36	kJ/mol	Joback Method
hvap	91.49	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.596		Crippen Method
mcvol	407.350	ml/mol	McGowan Method
pc	824.79	kPa	Joback Method
rinpol	3328.00		NIST Webbook
tb	1027.55	K	Joback Method
tc	1261.86	K	Joback Method
tf	581.33	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1577.50	J/mol×K	1027.55	Joback Method
cpg	1612.85	J/mol×K	1066.60	Joback Method
cpg	1649.02	J/mol×K	1105.65	Joback Method
cpg	1686.40	J/mol×K	1144.70	Joback Method
cpg	1725.34	J/mol×K	1183.75	Joback Method
cpg	1766.19	J/mol×K	1222.81	Joback Method
cpg	1809.32	J/mol×K	1261.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110717&Units=SI
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

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