24-Methyl-31-norcycloartenol acetate

Inchi: InChI=1S/C32H52O2/c1-20(2)21(3)9-10-22(4)24-11-12-25-26-13-14-27-29(6,7)28(34-23
InchiKey: NRTONKDGIFSFHT-CQOVQXQESA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CC=C(C)C(C)C)CCC2C4CCC3C1(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	266.08	kJ/mol	Joback Method
hf	-526.62	kJ/mol	Joback Method
hfus	36.74	kJ/mol	Joback Method
hvap	89.48	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	866.07	kPa	Joback Method
rinpol	3430.00		NIST Webbook
tb	1039.80	K	Joback Method
tc	1280.87	K	Joback Method
tf	631.30	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1657.01	J/mol×K	1039.80	Joback Method
cpg	1710.34	J/mol×K	1079.98	Joback Method
cpg	1768.24	J/mol×K	1120.16	Joback Method
cpg	1831.40	J/mol×K	1160.33	Joback Method
cpg	1900.55	J/mol×K	1200.51	Joback Method
cpg	1976.40	J/mol×K	1240.69	Joback Method
cpg	2059.68	J/mol×K	1280.87	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=R110440&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