24-Methyl-31-nor-23-dehydrocycloartanol acetate

Inchi: InChI=1S/C32H54O2/c1-20(2)21(3)9-10-22(4)24-11-12-25-26-13-14-27-29(6,7)28(34-23
InchiKey: ZJXWFABXIPUCGK-MNTLUMBWSA-N
Formula: C32H54O2
SMILES: CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CCC(C)C(C)C)CCC2C4CCC3C1(C)C
Mol. weight [g/mol]: 470.77

Physical Properties

Property code	Value	Unit	Source
gf	191.97	kJ/mol	Joback Method
hf	-639.33	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	89.06	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	8.675		Crippen Method
mcvol	414.880	ml/mol	McGowan Method
pc	841.62	kPa	Joback Method
rinpol	3374.00		NIST Webbook
tb	1035.32	K	Joback Method
tc	1273.15	K	Joback Method
tf	635.34	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1682.71	J/mol×K	1035.32	Joback Method
cpg	1734.65	J/mol×K	1074.96	Joback Method
cpg	1790.69	J/mol×K	1114.60	Joback Method
cpg	1851.50	J/mol×K	1154.24	Joback Method
cpg	1917.75	J/mol×K	1193.87	Joback Method
cpg	1990.11	J/mol×K	1233.51	Joback Method
cpg	2069.25	J/mol×K	1273.15	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=R110415&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