24-Methylenecycloartanol acetate

Inchi: InChI=1S/C33H52O2/c1-21(2)22(3)10-11-23(4)25-14-16-31(9)27-13-12-26-29(6,7)28(35-
InchiKey: NSVYRGOREINNBF-WKOZSBMGSA-N
Formula: C33H52O2
SMILES: C=C(CCC(C)C1CCC2(C)C3=CCC4C(C)(C)C(OC(C)=O)CCC45CC35CCC12C)C(C)C
Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	304.67	kJ/mol	Joback Method
hf	-457.16	kJ/mol	Joback Method
hfus	31.31	kJ/mol	Joback Method
hvap	91.19	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	8.906		Crippen Method
mcvol	420.370	ml/mol	McGowan Method
pc	862.51	kPa	Joback Method
rinpol	3443.00		NIST Webbook
tb	1064.25	K	Joback Method
tc	1308.94	K	Joback Method
tf	687.31	K	Joback Method
vc	1.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1718.01	J/mol×K	1064.25	Joback Method
cpg	1782.41	J/mol×K	1105.03	Joback Method
cpg	1853.47	J/mol×K	1145.81	Joback Method
cpg	1932.05	J/mol×K	1186.60	Joback Method
cpg	2019.01	J/mol×K	1227.38	Joback Method
cpg	2115.22	J/mol×K	1268.16	Joback Method
cpg	2221.55	J/mol×K	1308.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R489875&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

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