31-Norcycloartanol acetate

Inchi: InChI=1S/C31H52O2/c1-20(2)9-8-10-21(3)23-11-12-24-25-13-14-26-28(5,6)27(33-22(4)3
InchiKey: OQKCUVXEGARQNX-HFCUEOPBSA-N
Formula: C31H52O2
SMILES: CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CCCC(C)C)CCC2C4CCC3C1(C)C
Mol. weight [g/mol]: 456.74

Physical Properties

Property code	Value	Unit	Source
gf	185.99	kJ/mol	Joback Method
hf	-613.41	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	87.22	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	8.429		Crippen Method
mcvol	400.790	ml/mol	McGowan Method
pc	886.30	kPa	Joback Method
rinpol	3289.00		NIST Webbook
rinpol	3289.00		NIST Webbook
tb	1012.88	K	Joback Method
tc	1247.90	K	Joback Method
tf	639.07	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1602.50	J/mol×K	1012.88	Joback Method
cpg	1651.07	J/mol×K	1052.05	Joback Method
cpg	1703.34	J/mol×K	1091.22	Joback Method
cpg	1759.95	J/mol×K	1130.39	Joback Method
cpg	1821.54	J/mol×K	1169.56	Joback Method
cpg	1888.75	J/mol×K	1208.73	Joback Method
cpg	1962.22	J/mol×K	1247.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110653&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