Epibauerenol (7-baueren-3A-ol) acetate

Inchi: InChI=1S/C32H52O2/c1-20-12-15-29(6)18-19-31(8)24-10-11-25-28(4,5)26(34-22(3)33)14
InchiKey: DTHUXXMWYWKQKX-WXUJXVDFSA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC2(C)C3CCC4(C)C5C(C)C(C)CCC5(C)CCC4(C)C3=CCC2C1(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	150.31	kJ/mol	Joback Method
hf	-627.26	kJ/mol	Joback Method
hfus	33.17	kJ/mol	Joback Method
hvap	90.10	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	3364.00		NIST Webbook
tb	1048.76	K	Joback Method
tc	1298.05	K	Joback Method
tf	694.96	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1696.11	J/mol×K	1048.76	Joback Method
cpg	1756.43	J/mol×K	1090.31	Joback Method
cpg	1822.21	J/mol×K	1131.86	Joback Method
cpg	1894.24	J/mol×K	1173.40	Joback Method
cpg	1973.35	J/mol×K	1214.95	Joback Method
cpg	2060.35	J/mol×K	1256.50	Joback Method
cpg	2156.06	J/mol×K	1298.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111136&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