24(28)-Dihydroobtusifoliol acetate

Inchi: InChI=1S/C32H54O2/c1-20(2)21(3)10-11-22(4)25-14-18-32(9)28-13-12-26-23(5)29(34-2
InchiKey: AEUXNTWFROSOOS-AYUWEKAFSA-N
Formula: C32H54O2
SMILES: CC(=O)OC1CCC2(C)C3=C(CCC2C1C)C1(C)CCC(C(C)CCC(C)C(C)C)C1(C)CC3
Mol. weight [g/mol]: 470.77

Physical Properties

Property code	Value	Unit	Source
gf	130.92	kJ/mol	Joback Method
hf	-684.51	kJ/mol	Joback Method
hfus	37.66	kJ/mol	Joback Method
hvap	92.57	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.986		Crippen Method
mcvol	421.440	ml/mol	McGowan Method
pc	801.15	kPa	Joback Method
rinpol	3336.00		NIST Webbook
rinpol	3336.00		NIST Webbook
tb	1050.67	K	Joback Method
tc	1289.34	K	Joback Method
tf	616.50	K	Joback Method
vc	1.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1665.41	J/mol×K	1050.67	Joback Method
cpg	1709.67	J/mol×K	1090.45	Joback Method
cpg	1756.37	J/mol×K	1130.23	Joback Method
cpg	1806.02	J/mol×K	1170.01	Joback Method
cpg	1859.12	J/mol×K	1209.79	Joback Method
cpg	1916.15	J/mol×K	1249.56	Joback Method
cpg	1977.62	J/mol×K	1289.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110188&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