Obtusifoliol acetate

Inchi: InChI=1S/C32H52O2/c1-20(2)21(3)10-11-22(4)25-14-18-32(9)28-13-12-26-23(5)29(34-2
InchiKey: QZHIABMWLYKDJA-HTDQBKTMSA-N
Formula: C32H52O2
SMILES: C=C(CCC(C)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(OC(C)=O)C(C)C1CC3)C(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	212.65	kJ/mol	Joback Method
hf	-563.59	kJ/mol	Joback Method
hfus	38.59	kJ/mol	Joback Method
hvap	92.36	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.906		Crippen Method
mcvol	417.140	ml/mol	McGowan Method
pc	819.13	kPa	Joback Method
rinpol	3328.00		NIST Webbook
tb	1047.67	K	Joback Method
tc	1286.79	K	Joback Method
tf	615.78	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1632.41	J/mol×K	1047.67	Joback Method
cpg	1676.36	J/mol×K	1087.52	Joback Method
cpg	1722.87	J/mol×K	1127.38	Joback Method
cpg	1772.44	J/mol×K	1167.23	Joback Method
cpg	1825.58	J/mol×K	1207.08	Joback Method
cpg	1882.79	J/mol×K	1246.93	Joback Method
cpg	1944.59	J/mol×K	1286.79	Joback Method

Sources

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=R111374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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