Isoarborinol (9[11]-arborinenol) acetate

Inchi: InChI=1S/C32H50O2/c1-20(2)22-10-13-26-30(22,7)18-19-31(8)24-11-12-25-28(4,5)27(34
InchiKey: HGJARKCTVXMQKJ-OHLBPESASA-N
Formula: C32H50O2
SMILES: C=C(C)C1CCC2C1(C)CCC1(C)C3CCC4C(C)(CCC(OC(C)=O)C4(C)C)C3=CCC21C
Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	249.41	kJ/mol	Joback Method
hf	-485.12	kJ/mol	Joback Method
hfus	31.61	kJ/mol	Joback Method
hvap	89.64	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	8.516		Crippen Method
mcvol	406.280	ml/mol	McGowan Method
pc	909.43	kPa	Joback Method
rinpol	3468.00		NIST Webbook
tb	1045.72	K	Joback Method
tc	1295.30	K	Joback Method
tf	687.00	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1654.61	J/mol×K	1045.72	Joback Method
cpg	1715.01	J/mol×K	1087.32	Joback Method
cpg	1781.25	J/mol×K	1128.91	Joback Method
cpg	1854.17	J/mol×K	1170.51	Joback Method
cpg	1934.63	J/mol×K	1212.11	Joback Method
cpg	2023.47	J/mol×K	1253.70	Joback Method
cpg	2121.55	J/mol×K	1295.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111270&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