Isomultiflorenol (8-multiflorenenol) acetate

Inchi: InChI=1S/C32H52O2/c1-21(33)34-26-13-14-30(7)22-12-15-32(9)25-20-27(2,3)16-17-29(
InchiKey: IQPSCJJRYFMIOC-JWPJBSNZSA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC2(C)C3=C(CCC2C1(C)C)C1(C)CCC2(C)CCC(C)(C)CC2C1(C)CC3
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	150.61	kJ/mol	Joback Method
hf	-582.81	kJ/mol	Joback Method
hfus	24.34	kJ/mol	Joback Method
hvap	90.22	kJ/mol	Joback Method
log10ws	-9.59		Crippen Method
logp	8.884		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	3360.00		NIST Webbook
tb	1063.32	K	Joback Method
tc	1318.07	K	Joback Method
tf	739.86	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1717.06	J/mol×K	1063.32	Joback Method
cpg	1789.03	J/mol×K	1105.78	Joback Method
cpg	1868.87	J/mol×K	1148.24	Joback Method
cpg	1957.61	J/mol×K	1190.69	Joback Method
cpg	2056.25	J/mol×K	1233.15	Joback Method
cpg	2165.81	J/mol×K	1275.61	Joback Method
cpg	2287.33	J/mol×K	1318.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111309&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