Fernenol (9[11]-fernenol) acetate

Inchi: InChI=1S/C32H52O2/c1-20(2)22-10-13-26-30(22,7)18-19-31(8)24-11-12-25-28(4,5)27(34
InchiKey: WQWTUUFHPFYTRZ-OHLBPESASA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC2(C)C3=CCC4(C)C5CCC(C(C)C)C5(C)CCC4(C)C3CCC2C1(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	167.68	kJ/mol	Joback Method
hf	-606.04	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	3437.00		NIST Webbook
rinpol	3437.00		NIST Webbook
tb	1048.72	K	Joback Method
tc	1296.76	K	Joback Method
tf	687.72	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1688.55	J/mol×K	1048.72	Joback Method
cpg	1749.18	J/mol×K	1090.06	Joback Method
cpg	1815.48	J/mol×K	1131.40	Joback Method
cpg	1888.28	J/mol×K	1172.74	Joback Method
cpg	1968.41	J/mol×K	1214.08	Joback Method
cpg	2056.69	J/mol×K	1255.42	Joback Method
cpg	2153.95	J/mol×K	1296.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111210&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

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