Pentadeca-2,5E,13-triene, 7-acetoxymethyl-2,6,10,14-tetramethyl-10-17-epox (Peucelinenoxide acetate)

Inchi: InChI=1S/C22H36O3/c1-17(2)9-7-11-20-16-25-22(6,13-8-10-18(3)4)14-12-21(20)15-24-1
InchiKey: HWOJVASMJVEOSP-RGVLZGJSSA-N
Formula: C22H36O3
SMILES: CC(=O)OCC1CCC(C)(CCC=C(C)C)OCC1=CCC=C(C)C
Mol. weight [g/mol]: 348.52

Physical Properties

Property code	Value	Unit	Source
gf	2.27	kJ/mol	Joback Method
hf	-540.26	kJ/mol	Joback Method
hfus	46.12	kJ/mol	Joback Method
hvap	78.24	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.764		Crippen Method
mcvol	310.390	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook
tb	840.11	K	Joback Method
tc	1051.97	K	Joback Method
tf	432.23	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.77	J/mol×K	840.11	Joback Method
cpg	1014.58	J/mol×K	875.42	Joback Method
cpg	1035.64	J/mol×K	910.73	Joback Method
cpg	1056.11	J/mol×K	946.04	Joback Method
cpg	1076.10	J/mol×K	981.35	Joback Method
cpg	1095.77	J/mol×K	1016.66	Joback Method
cpg	1115.25	J/mol×K	1051.97	Joback Method

Sources

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=R604425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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