2-Pentenoic acid, 5-(decahydro-5,5,8a-trimethyl-2-methylene-1-naph
methyl ester, [1R-[1«alpha»(E),4a«beta»,8a«alpha»]]-

Other names: 5«beta»,9«beta»H,10«alpha»-Labda-8(20),13-dien-15-oic acid, methyl ester, (E)-
Methyl copalate
Methyl ester of 5«beta»,9«beta»,10«alpha»-Labda-8(20),13-dien-15-oic acid (isomer A)
(E)-Methyl 3-methyl-5-((1R,4aR,8aR)-5,5,8a-trimethyl-2-methylenedecahydronaphthalen-1-yl)pent-2

Inchi: InChI=1S/C21H34O2/c1-15(14-19(22)23-6)8-10-17-16(2)9-11-18-20(3,4)12-7-13-21(17,1

InchiKey: KYTKOCVFNCZSSC-CCEZHUSRSA-N

Formula: C21H34O2

SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1CCC(C)=CC(=O)OC

Mol. weight [g/mol]: 318.49

CAS: 17110-88-2

Physical Properties

Property code	Value	Unit	Source
gf	63.47	kJ/mol	Joback Method
hf	-419.14	kJ/mol	Joback Method
hfus	28.08	kJ/mol	Joback Method
hvap	69.29	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.685		Crippen Method
mcvol	283.870	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	2326.60		NIST Webbook
rinpol	2312.00		NIST Webbook
rinpol	2326.60		NIST Webbook
tb	781.07	K	Joback Method
tc	998.73	K	Joback Method
tf	454.35	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.66	J/mol×K	781.07	Joback Method
cpg	924.60	J/mol×K	817.35	Joback Method

cpg	948.03	J/mol×K	853.62	Joback Method
cpg	971.18	J/mol×K	889.90	Joback Method
cpg	994.27	J/mol×K	926.18	Joback Method
cpg	1017.54	J/mol×K	962.46	Joback Method
cpg	1041.22	J/mol×K	998.73	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=C17110882&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