1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydro-1,4a-dimethyl-, methyl ester, [1R-(1«alpha»,4a«beta»,4b«alpha»,7«alpha»,10a«alpha»)]-

Other names: Podocarp-7-en-15-oic acid, 13«beta»-methyl-13-vinyl-, methyl ester
Isopimaric acid, methyl ester
Methyl isopimarate

Inchi: InChI=1S/C21H32O2/c1-6-19(2)13-10-16-15(14-19)8-9-17-20(16,3)11-7-12-21(17,4)18(2

InchiKey: QMZKBAQNFAMESG-RUSYTGNQSA-N

Formula: C21H32O2

SMILES: C=CC1(C)CCC2C(=CCC3C(C)(C(=O)OC)CCCC23C)C1

Mol. weight [g/mol]: 316.48

CAS: 1686-62-0

Physical Properties

Property code	Value	Unit	Source
gf	90.05	kJ/mol	Joback Method
hf	-357.19	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	68.31	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.295		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2289.00		NIST Webbook
rinpol	2297.00		NIST Webbook
rinpol	2299.00		NIST Webbook
rinpol	2271.00		NIST Webbook
rinpol	2297.00		NIST Webbook
rinpol	2271.00		NIST Webbook
rinpol	2284.00		NIST Webbook
rinpol	2297.00		NIST Webbook
ripol	2876.00		NIST Webbook
ripol	2875.00		NIST Webbook
tb	789.94	K	Joback Method
tc	1026.62	K	Joback Method
tf	509.55	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.46	J/mol×K	789.94	Joback Method
cpg	910.70	J/mol×K	829.39	Joback Method
cpg	937.05	J/mol×K	868.83	Joback Method
cpg	963.92	J/mol×K	908.28	Joback Method
cpg	991.75	J/mol×K	947.73	Joback Method
cpg	1020.95	J/mol×K	987.17	Joback Method
cpg	1051.97	J/mol×K	1026.62	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1686620&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume