1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,10a-hexahydro-1,4a-dimethyl-7-(1-meth
methyl ester, [1R-(1«alpha»,4a«beta»,10a«alpha»)]-

Other names: Podocarpa-6,8,11,13-tetraen-15-oic acid, 13-isopropyl-, methyl ester
Methyl 6-dehydrodehydroabietate
Methyl 6,8,11,13-abietatetraen-18-oate
Inchi: InChI=1S/C21H28O2/c1-14(2)15-7-9-17-16(13-15)8-10-18-20(17,3)11-6-12-21(18,4)19(2
InchiKey: GNEXBBYESLSHNT-UHFFFAOYSA-N
Formula: C21H28O2
SMILES: COC(=O)C1(C)CCCC2(C)c3ccc(C(C)C)cc3C=CC12
Mol. weight [g/mol]: 312.45
CAS: 18492-76-7

Physical Properties

Property code	Value	Unit	Source
gf	91.30	kJ/mol	Joback Method
hf	-312.06	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	72.56	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.074		Crippen Method
mcvol	264.410	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	2378.00		NIST Webbook
tb	809.36	K	Joback Method
tc	1045.35	K	Joback Method
tf	508.21	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.82	J/mol×K	809.36	Joback Method
cpg	851.28	J/mol×K	848.69	Joback Method
cpg	873.61	J/mol×K	888.02	Joback Method
cpg	896.12	J/mol×K	927.36	Joback Method
cpg	919.13	J/mol×K	966.69	Joback Method

cpg	942.95	J/mol×K	1006.02	Joback Method
cpg	967.90	J/mol×K	1045.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18492767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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