1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,4a-dim
methyl ester, [1R-(1«alpha»,4a«beta»,4b«alpha»,10a«alpha»)]-

Other names: Podocarp-8(14)-en-15-oic acid, 13-isopropylidene-, methyl ester
Methyl neoabietate
Neoabietic acid, methyl ester
Inchi: InChI=1S/C21H32O2/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: XLNYKQDSHLEWFW-QDDLRWIDSA-N
Formula: C21H32O2
SMILES: COC(=O)C1(C)CCCC2(C)C3CCC(=C(C)C)C=C3CCC12
Mol. weight [g/mol]: 316.48
CAS: 3310-97-2

Physical Properties

Property code	Value	Unit	Source
gf	52.32	kJ/mol	Joback Method
hf	-411.28	kJ/mol	Joback Method
hfus	25.16	kJ/mol	Joback Method
hvap	71.31	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.439		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	2387.00		NIST Webbook
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
rinpol	2387.00		NIST Webbook
rinpol	2397.00		NIST Webbook
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
ripol	3055.00		NIST Webbook
ripol	3062.00		NIST Webbook
tb	804.21	K	Joback Method
tc	1038.48	K	Joback Method
tf	488.05	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.02	J/mol×K	804.21	Joback Method
cpg	911.81	J/mol×K	843.25	Joback Method
cpg	936.26	J/mol×K	882.30	Joback Method
cpg	960.68	J/mol×K	921.34	Joback Method
cpg	985.40	J/mol×K	960.39	Joback Method
cpg	1010.72	J/mol×K	999.43	Joback Method
cpg	1036.95	J/mol×K	1038.48	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=C3310972&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume