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

Other names:	Methyl 7,13,15-abietatrienoate
	Methyl 7,13,15-Abietatrien-18-oate
Inchi:	InChI=1S/C21H30O2/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:	VFWGUFBDEBVPBM-UHFFFAOYSA-N
Formula:	C21H30O2
SMILES:	C=C(C)C1=CC2=CCC3C(C)(C(=O)OC)CCCC3(C)C2CC1
Mol. weight [g/mol]:	314.46
CAS:	54850-32-7

Physical Properties

Property code	Value	Unit	Source
gf	115.03	kJ/mol	Joback Method
hf	-315.57	kJ/mol	Joback Method
hfus	24.39	kJ/mol	Joback Method
hvap	70.80	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.215		Crippen Method
mcvol	268.710	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2466.00		NIST Webbook
rinpol	2492.00		NIST Webbook
rinpol	2492.00		NIST Webbook
rinpol	2466.00		NIST Webbook
tb	798.39	K	Joback Method
tc	1033.52	K	Joback Method
tf	489.21	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.98	J/mol×K	798.39	Joback Method
cpg	882.95	J/mol×K	837.58	Joback Method
cpg	906.59	J/mol×K	876.77	Joback Method

cpg	930.20	J/mol×K	915.95	Joback Method
cpg	954.10	J/mol×K	955.14	Joback Method
cpg	978.61	J/mol×K	994.33	Joback Method
cpg	1004.03	J/mol×K	1033.52	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=C54850327&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