Methyl dehydroabietate

Other names:	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1«alpha»,4a«beta»,10a«alpha»)]- Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl-, methyl ester Methyl 8,11,13-abietatrien-18-oate 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, (1R,4aS,10aR)- Dehydroabietic acid methyl ester Phenanthrene-1-carboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-7-isopropyl-1,4a-dimethyl-, methyl ester, , [1R-(1«alpha»,4a«beta»,10a«alpha»)]- Methyl abieta-8,11,13-trien-18-oate NSC 146198 NSC 81596
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:	PGZCJOPTDHWYES-UHFFFAOYSA-N
Formula:	C21H30O2
SMILES:	COC(=O)C1(C)CCCC2(C)c3ccc(C(C)C)cc3CCC12
Mol. weight [g/mol]:	314.46
CAS:	1235-74-1

Physical Properties

Property code	Value	Unit	Source
gf	61.34	kJ/mol	Joback Method
hf	-369.84	kJ/mol	Joback Method
hfus	23.22	kJ/mol	Joback Method
hvap	72.27	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.993		Crippen Method
mcvol	268.710	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	2333.00		NIST Webbook
rinpol	2336.00		NIST Webbook
rinpol	2338.00		NIST Webbook
rinpol	2361.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	388.30		NIST Webbook
rinpol	2354.50		NIST Webbook
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
rinpol	2324.00		NIST Webbook
rinpol	2359.60		NIST Webbook

rinpol	2304.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2293.00		NIST Webbook
rinpol	388.30		NIST Webbook
ripol	3016.00		NIST Webbook
ripol	3016.00		NIST Webbook
tb	810.20	K	Joback Method
tc	1044.45	K	Joback Method
tf	335.50 ± 0.50	K	NIST Webbook
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.31	J/mol×K	810.20	Joback Method
cpg	879.62	J/mol×K	849.24	Joback Method
cpg	902.74	J/mol×K	888.28	Joback Method
cpg	925.96	J/mol×K	927.33	Joback Method
cpg	949.61	J/mol×K	966.37	Joback Method
cpg	973.97	J/mol×K	1005.41	Joback Method
cpg	999.36	J/mol×K	1044.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.00 ± 1.00	K	0.03	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1235741&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume