Methyl abietate

Other names:	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1«alpha»,4a«beta»,4b«alpha»,10a«alpha»)]- Podocarpa-7,13-dien-15-oic acid, 13-isopropyl-, methyl ester Abietic acid, methyl ester Methyl 7,13-abietadien-18-oate Wood rosin, methyl ester 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, (1R,4aR,4bR,10aR)- NSC 2141
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:	OVXRPXGVKBHGQO-QDDLRWIDSA-N
Formula:	C21H32O2
SMILES:	COC(=O)C1(C)CCCC2(C)C3CCC(C(C)C)=CC3=CCC12
Mol. weight [g/mol]:	316.48
CAS:	127-25-3

Physical Properties

Property code	Value	Unit	Source
gf	33.30	kJ/mol	Joback Method
hf	-436.49	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	71.00	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.295		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2393.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2344.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2339.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2356.00		NIST Webbook
ripol	3016.00		NIST Webbook
ripol	3016.00		NIST Webbook
ripol	3016.00		NIST Webbook
tb	801.39	K	Joback Method
tc	1033.26	K	Joback Method

tf	489.93	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.67	J/mol×K	801.39	Joback Method
cpg	911.14	J/mol×K	840.03	Joback Method
cpg	935.22	J/mol×K	878.68	Joback Method
cpg	959.20	J/mol×K	917.32	Joback Method
cpg	983.38	J/mol×K	955.97	Joback Method
cpg	1008.04	J/mol×K	994.61	Joback Method
cpg	1033.50	J/mol×K	1033.26	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=C127253&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

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