1-Phenanthrenecarboxylic acid, 7-ethyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,4 methyl ester, [1R-(1«alpha»,4a«beta»,7«beta»,10a«alpha»)]-

Other names:	Podocarp-8-en-15-oic acid, 13«beta»-ethyl-13-methyl-, methyl ester
	Methyl 8-pimaren-18-oate
Inchi:	InChI=1S/C21H34O2/c1-6-19(2)13-10-16-15(14-19)8-9-17-20(16,3)11-7-12-21(17,4)18(2
InchiKey:	LZUSHGHGVLPXFI-UHFFFAOYSA-N
Formula:	C21H34O2
SMILES:	CCC1(C)CCC2=C(CCC3C(C)(C(=O)OC)CCCC23C)C1
Mol. weight [g/mol]:	318.49
CAS:	3582-25-0

Physical Properties

Property code	Value	Unit	Source
gf	0.29	kJ/mol	Joback Method
hf	-473.75	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.663		Crippen Method
mcvol	277.310	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	802.91	K	Joback Method
tc	1036.25	K	Joback Method
tf	528.07	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.00	J/mol×K	802.91	Joback Method
cpg	935.45	J/mol×K	841.80	Joback Method
cpg	962.13	J/mol×K	880.69	Joback Method
cpg	989.43	J/mol×K	919.58	Joback Method
cpg	1017.77	J/mol×K	958.47	Joback Method

cpg	1047.55	J/mol×K	997.36	Joback Method
cpg	1079.16	J/mol×K	1036.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3582250&Units=SI

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