1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-m [1S-(1«alpha»,4a«alpha»,10a«beta»)]-

Other names:	Podocarpa-8,11,13-trien-16-al, 13-isopropyl- 4-Epiabietal, dehydro- (1S,4aS,10aR)-7-Isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-
Inchi:	InChI=1S/C20H28O/c1-14(2)15-6-8-17-16(12-15)7-9-18-19(3,13-21)10-5-11-20(17,18)4/
InchiKey:	YCLCHPWRGSDZKL-UHFFFAOYSA-N
Formula:	C20H28O
SMILES:	CC(C)c1ccc2c(c1)CCC1C(C)(C=O)CCCC21C
Mol. weight [g/mol]:	284.44
CAS:	24035-50-5

Physical Properties

Property code	Value	Unit	Source
gf	187.32	kJ/mol	Joback Method
hf	-189.98	kJ/mol	Joback Method
hfus	20.13	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.019		Crippen Method
mcvol	248.750	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	2289.20		NIST Webbook
rinpol	2289.20		NIST Webbook
tb	759.69	K	Joback Method
tc	996.72	K	Joback Method
tf	466.02	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.98	J/mol×K	759.69	Joback Method
cpg	787.50	J/mol×K	799.19	Joback Method
cpg	809.58	J/mol×K	838.70	Joback Method
cpg	831.56	J/mol×K	878.20	Joback Method

cpg	853.76	J/mol×K	917.71	Joback Method
cpg	876.53	J/mol×K	957.21	Joback Method
cpg	900.19	J/mol×K	996.72	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=C24035505&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