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

Other names: (1R,4aR,4bS,10aR)-1,4a-Dimethyl-7-(propan-2-ylidene)-1,2,3,4,4a,4b,5,6,7,9,10,10a-doc
Podocarp-8(14)-en-15-oic acid, 13-isopropylidene-
acid
Neoabietic acid

Inchi: InChI=1S/C20H30O2/c1-13(2)14-6-8-16-15(12-14)7-9-17-19(16,3)10-5-11-20(17,4)18(21

InchiKey: KGMSWPSAVZAMKR-UHFFFAOYSA-N

Formula: C20H30O2

SMILES: CC(C)=C1C=C2CCC3C(C)(C(=O)O)CCCC3(C)C2CC1

Mol. weight [g/mol]: 302.45

CAS: 471-77-2

Physical Properties

Property code	Value	Unit	Source
gf	12.08	kJ/mol	Joback Method
hf	-410.65	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	83.35	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.350		Crippen Method
mcvol	258.920	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	851.09	K	Joback Method
tc	1076.87	K	Joback Method
tf	515.37	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.76	J/mol×K	851.09	Joback Method
cpg	891.18	J/mol×K	888.72	Joback Method
cpg	913.79	J/mol×K	926.35	Joback Method
cpg	936.86	J/mol×K	963.98	Joback Method

cpg	960.71	J/mol×K	1001.61	Joback Method
cpg	985.62	J/mol×K	1039.24	Joback Method
cpg	1011.90	J/mol×K	1076.87	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=C471772&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