Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydr
[4aS-(4a«alpha»,4b«beta»,7«beta»,10a«beta»)]-

Other names: Podocarp-8(14)-ene, 13«beta»-methyl-13-vinyl-
Sandaracopimaradiene
13-Isopimaradiene
8(14),15-Sandaracopimaradiene
Sandaracopimara-8(14),15-diene
Pimara-8(14),15-diene

Inchi: InChI=1S/C20H32/c1-6-19(4)13-10-16-15(14-19)8-9-17-18(2,3)11-7-12-20(16,17)5/h6,14

InchiKey: XDSYKASBVOZOAG-WXDAQCLHSA-N

Formula: C20H32

SMILES: C=CC1(C)C=C2CCC3C(C)(C)CCCC3(C)C2CC1

Mol. weight [g/mol]: 272.47

CAS: 1686-56-2

Physical Properties

Property code	Value	Unit	Source
gf	315.55	kJ/mol	Joback Method
hf	-91.75	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	56.93	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	6.142		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1946.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1969.00		NIST Webbook
rinpol	1951.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1935.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1943.00		NIST Webbook

rinpol	1969.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	1969.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1967.00		NIST Webbook
rinpol	1973.40		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1935.00		NIST Webbook
rinpol	1941.00		NIST Webbook
ripol	2243.00		NIST Webbook
ripol	2243.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2229.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2279.00		NIST Webbook
tb	690.77	K	Joback Method
tc	930.20	K	Joback Method
tf	426.12	K	Joback Method

vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.71	J/mol×K	690.77	Joback Method
cpg	789.62	J/mol×K	730.67	Joback Method
cpg	815.66	J/mol×K	770.58	Joback Method
cpg	841.30	J/mol×K	810.48	Joback Method
cpg	867.00	J/mol×K	850.39	Joback Method
cpg	893.21	J/mol×K	890.29	Joback Method
cpg	920.40	J/mol×K	930.20	Joback Method

Sources

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=C1686562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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