

Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydro [4aS-(4a«alpha»,4b«beta»,7«beta»,10a«beta»)]-

Other names: Podocarp-7-ene, 13«beta»-methyl-13-vinyl-Isopimar-7,15-diene

Isopimaradiene

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/h6,8,10,11,13,14,16,17,19,20
InchiKey: VCOVNILQQZROK-WXDAQCLHSA-N
Formula: C20H32
SMILES: C=CC1(C)CCC2C(=CCC3C(C)(C)CCCC23C)C1
Mol. weight [g/mol]: 272.47
CAS: 1686-66-4

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	1999.00		NIST Webbook
rinpol	1969.00		NIST Webbook
rinpol	2013.00		NIST Webbook
rinpol	1969.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1968.00		NIST Webbook
ripol	2332.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2319.00		NIST Webbook
ripol	2346.00		NIST Webbook
ripol	2349.00		NIST Webbook
ripol	2349.00		NIST Webbook
ripol	2335.00		NIST Webbook
tb	690.77	K	Joback Method
tc	930.20	K	Joback Method

tf	426.12	K	Joback Method
vc	0.946	m ³ /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

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=C1686664&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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