Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,8a,9-dodecahydro-1,1,4b,7-tetramethyl-, [4aS-(4a«alpha»,4b«beta»,7«alpha»,8a«alpha»)]-

Other names:	Rimuen Rimuene 5,15-Rosadiene Rosa-5,15-diene, (13S)- Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,8a,9-dodecahydro-1,1,4b,7-tetramethyl-, (4aS,4bR,7S,8aR)- Rosa-5,15-diene, (4aS,4bR,7S,8aR)-
Inchi:	InChI=1S/C20H32/c1-6-19(4)12-13-20(5)15(14-19)9-10-16-17(20)8-7-11-18(16,2)3/h6,10
InchiKey:	BAIWMJSLFJWAQP-LYBGUNNDSA-N
Formula:	C20H32
SMILES:	C=CC1(C)CCC2(C)C(CC=C3C2CCCC3(C)C)C1
Mol. weight [g/mol]:	272.47
CAS:	1686-67-5

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	1926.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1901.90		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1906.00		NIST Webbook
rinpol	1914.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1930.00		NIST Webbook

rinpol	1894.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1901.90		NIST Webbook
rinpol	1886.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2187.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2233.00		NIST Webbook
ripol	2232.00		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: 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=C1686675&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume