(R,1E,5E,9E)-1,5,9-Trimethyl-12-(prop-1-en-2-yl)cy

Other names: 1,5,9-Cyclotetradecatriene, 1,5,9-trimethyl-12-(1-methylethenyl)-, (1E,5E,9E,12R)-
1,5,9-Cyclotetradecatriene, 1,5,9-trimethyl-12-(1-methylethenyl)-, [R-(E,E,E)]-
1,5,9-Cyclotetradecatriene, 13-isopropenyl-2,6,10-trimethyl-, (-)-
(-)-Cembrene A
Cembrene A
Neocembrene A
(R)-(-)-Cembrene A
Neocembrene
CEMBRENE A (711293 K111)
3E-Cembrene A
(E)-3-Cembrene A

Inchi: InChI=1S/C20H32/c1-16(2)20-14-12-18(4)10-6-8-17(3)9-7-11-19(5)13-15-20/h8,11-12,20

InchiKey: VWSPQDDPRITBAM-KPGNMOGWSA-N

Formula: C20H32

SMILES: C=C(C)C1CC=C(C)CCC=C(C)CCC=C(C)CC1

Mol. weight [g/mol]: 272.47

CAS: 31570-39-5

Physical Properties

Property code	Value	Unit	Source
gf	185.45	kJ/mol	Joback Method
hf	-196.52	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	64.19	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.762		Crippen Method
mcvol	264.600	ml/mol	McGowan Method
pc	1453.46	kPa	Joback Method
rinpol	1960.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1956.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1970.00		NIST Webbook

rinpol	1956.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1951.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1959.00		NIST Webbook
tb	719.69	K	Joback Method
tc	956.28	K	Joback Method
tf	318.50	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.61	J/mol×K	719.69	Joback Method
cpg	800.41	J/mol×K	759.12	Joback Method
cpg	825.14	J/mol×K	798.55	Joback Method
cpg	847.79	J/mol×K	837.98	Joback Method
cpg	868.34	J/mol×K	877.42	Joback Method
cpg	886.78	J/mol×K	916.85	Joback Method
cpg	903.08	J/mol×K	956.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31570395&Units=SI
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

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