1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(E,Z,E,E)]-

Other names: 1,3,6,10-Cyclotetradecatetraene, 14-isopropyl-3,7,11-trimethyl-, (+)-
(S,1E,3Z,6E,10E)-14-Isopropyl-3,7,11-trimethylcyclotetradeca-1,3,6,10-tetraene
Cembrene
Thunbergen
Thunbergene
(1S,2E,7E,11E)-2,4(18),7,11-Cembratraene

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

InchiKey: DMHADBQKVWXPPM-ZTAOLZRRSA-N

Formula: C20H32

SMILES: CC1=CCC=C(C)CCC=C(C)CCC(C(C)C)C=C1

Mol. weight [g/mol]: 272.47

CAS: 1898-13-1

Physical Properties

Property code	Value	Unit	Source
gf	133.68	kJ/mol	Joback Method
hf	-259.66	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	64.69	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	6.618		Crippen Method
mcvol	264.600	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	1947.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1958.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1929.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1951.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1935.00		NIST Webbook
rinpol	1929.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1939.00		NIST Webbook

rinpol	1930.00		NIST Webbook
rinpol	1948.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1923.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1932.00		NIST Webbook
ripol	2207.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2180.00		NIST Webbook
ripol	2181.00		NIST Webbook
tb	721.85	K	Joback Method
tc	956.66	K	Joback Method
tf	319.98	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.53	J/mol×K	721.85	Joback Method
cpg	800.86	J/mol×K	760.98	Joback Method
cpg	825.16	J/mol×K	800.12	Joback Method
cpg	847.39	J/mol×K	839.25	Joback Method
cpg	867.55	J/mol×K	878.39	Joback Method
cpg	885.60	J/mol×K	917.52	Joback Method
cpg	901.53	J/mol×K	956.66	Joback Method
dvisc	0.0041014	Pa×s	319.98	Joback Method
dvisc	0.0006090	Pa×s	386.96	Joback Method
dvisc	0.0001588	Pa×s	453.94	Joback Method
dvisc	0.0000585	Pa×s	520.91	Joback Method
dvisc	0.0000270	Pa×s	587.89	Joback Method
dvisc	0.0000146	Pa×s	654.87	Joback Method
dvisc	0.0000089	Pa×s	721.85	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=C1898131&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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