Cyclohexene, 6-ethenyl-6-methyl-1-(1-methylethyl)-3-(1-methyle (S)-

Other names: o-Menth-2-ene, 4-isopropylidene-1-vinyl-
«alpha»-Elemene
1-Isopropyl-6-methyl-3-(1-methylethylidene)-6-vinyl-1-cyclohexene-, (S)-
(S)-6-ethenyl-6-methyl-1-(1-methylethyl)-3-(1-methylethylidene)cyclohexene

Inchi: InChI=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,10,12H,1,8-9H2,2-6H3

InchiKey: QDUJKDRUFBJYSQ-UHFFFAOYSA-N

Formula: C15H24

SMILES: C=CC1(C)CCC(=C(C)C)C=C1C(C)C

Mol. weight [g/mol]: 204.35

CAS: 5951-67-7

Physical Properties

Property code	Value	Unit	Source
gf	237.02	kJ/mol	Joback Method
hf	-50.67	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	49.03	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	1431.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1477.00		NIST Webbook

rinpol	1486.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1469.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1687.00		NIST Webbook
tb	569.29	K	Joback Method
tc	782.44	K	Joback Method
tf	283.01	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.32	J/mol×K	569.29	Joback Method
cpg	512.66	J/mol×K	604.81	Joback Method
cpg	531.82	J/mol×K	640.34	Joback Method
cpg	549.95	J/mol×K	675.86	Joback Method
cpg	567.16	J/mol×K	711.39	Joback Method
cpg	583.58	J/mol×K	746.91	Joback Method
cpg	599.35	J/mol×K	782.44	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5951677&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

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