Cyclohexene, 1-methyl-4-(1-methylethyl)-

Other names:	1-Menthene
	1-Methyl-4-(1-methylethyl)cyclohexene
	1-Methyl-4-isopropyl-1-cyclohexene
	1-Methyl-4-isopropylcyclohexene
	1-p-Menthene
	4-Isopropyl-1-methyl-1-cyclohexene
	4-Isopropyl-1-methylcyclohexene
	Carvomenthene
	NSC 96749
	p-1-Menthene
	p-Ment-1-ene
	p-Menth-1-ene
	«delta»1-p-Menthene
	Â«deltaÂ»1-p-Menthene
Inchi:	InChI=1S/C10H18/c1-8(2)10-6-4-9(3)5-7-10/h4,8,10H,5-7H2,1-3H3
InchiKey:	FAMJUFMHYAFYNU-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	CC1=CCC(C(C)C)CC1
Mol. weight [g/mol]:	138.25
CAS:	5502-88-5

Physical Properties

Property code	Value	Unit	Source
chl	-6347.80 ± 3.10	kJ/mol	NIST Webbook
gf	75.66	kJ/mol	Joback Method
hf	-110.80 ± 3.20	kJ/mol	NIST Webbook
hfl	-159.80 ± 3.20	kJ/mol	NIST Webbook
hfus	10.80	kJ/mol	Joback Method
hvap	49.04 ± 0.33	kJ/mol	NIST Webbook
hvap	49.00	kJ/mol	NIST Webbook
log10ws	-3.27		Crippen Method
logp	3.389		Crippen Method
mcvol	136.600	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1017.00		NIST Webbook

rinpol	1020.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1019.90		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1005.70		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1017.70		NIST Webbook
rinpol	1032.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1146.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1146.00		NIST Webbook
tb	443.00 ± 5.00	K	NIST Webbook
tb	450.00 ± 1.00	K	NIST Webbook
tb	443.00 ± 4.00	K	NIST Webbook
tc	656.32	K	Joback Method
tf	208.12	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.78	J/mol×K	451.45	Joback Method
cpg	305.15	J/mol×K	485.59	Joback Method
cpg	322.63	J/mol×K	519.74	Joback Method

cpg	339.23	J/mol×K	553.88	Joback Method
cpg	354.99	J/mol×K	588.03	Joback Method
cpg	369.91	J/mol×K	622.17	Joback Method
cpg	384.04	J/mol×K	656.32	Joback Method
dvisc	0.0061732	Pa×s	208.12	Joback Method
dvisc	0.0022871	Pa×s	248.67	Joback Method
dvisc	0.0011194	Pa×s	289.23	Joback Method
dvisc	0.0006532	Pa×s	329.78	Joback Method
dvisc	0.0004288	Pa×s	370.34	Joback Method
dvisc	0.0003059	Pa×s	410.89	Joback Method
dvisc	0.0002319	Pa×s	451.45	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49226e+01
Coeff. B	-3.88885e+03
Coeff. C	-6.55970e+01
Temperature range (K), min.	331.32
Temperature range (K), max.	470.22

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5502885&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
pvap:	Vapor 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