Cyclohexene, 1-methyl-

Other names:	1-METHYL-1-CYCLOHEXENE
	1-Methylcyclohex-1-ene
	1-Methylcyclohexene
	1-Methylcyclohexene-1
	«alpha»-Methylcyclohexene
	Â«alphaÂ»-Methylcyclohexene
Inchi:	InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h5H,2-4,6H2,1H3
InchiKey:	CTMHWPIWNRWQEG-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC1=CCCCC1
Mol. weight [g/mol]:	96.17
CAS:	591-49-1

Physical Properties

Property code	Value	Unit	Source
affp	825.10	kJ/mol	NIST Webbook
basg	792.60	kJ/mol	NIST Webbook
chl	-4381.90	kJ/mol	NIST Webbook
chl	-4388.39 ± 0.67	kJ/mol	NIST Webbook
gf	60.55	kJ/mol	Joback Method
hf	-81.25 ± 0.79	kJ/mol	NIST Webbook
hfus	5.48	kJ/mol	Joback Method
hvap	37.50 ± 0.20	kJ/mol	NIST Webbook
hvap	37.80	kJ/mol	NIST Webbook
ie	8.69 ± 0.05	eV	NIST Webbook
ie	8.67 ± 0.02	eV	NIST Webbook
ie	8.67 ± 0.02	eV	NIST Webbook
log10ws	-3.27		Aqueous Solubility Prediction Method
log10ws	-3.27		Estimated Solubility Method
logp	2.507		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3569.00	kPa	KDB
rinpol	808.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	760.00		NIST Webbook

rinpol	773.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	766.40	NIST Webbook
rinpol	765.30	NIST Webbook
rinpol	763.90	NIST Webbook
rinpol	772.90	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	766.40	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	765.30	NIST Webbook
rinpol	763.90	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	769.30	NIST Webbook
rinpol	764.30	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	771.50	NIST Webbook

rinpol	768.50		NIST Webbook
rinpol	785.30		NIST Webbook
rinpol	780.40		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	766.40		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	761.70		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	758.50		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	767.00		NIST Webbook
ripol	932.00		NIST Webbook
ripol	914.90		NIST Webbook
ripol	900.00		NIST Webbook
ripol	932.00		NIST Webbook
ripol	900.00		NIST Webbook
ripol	909.00		NIST Webbook
ripol	923.10		NIST Webbook
ripol	914.90		NIST Webbook
ripol	931.70		NIST Webbook
ripol	923.10		NIST Webbook
ripol	914.90		NIST Webbook
ripol	931.70		NIST Webbook
ripol	932.00		NIST Webbook
ripol	906.00		NIST Webbook
ripol	909.00		NIST Webbook
ripol	923.00		NIST Webbook
ripol	915.00		NIST Webbook
tb	383.00 ± 4.00	K	NIST Webbook

tb	383.00 ± 2.00	K	NIST Webbook
tb	382.00 ± 6.00	K	NIST Webbook
tb	378.00 ± 5.00	K	NIST Webbook
tb	376.00 ± 16.00	K	NIST Webbook
tb	378.00 ± 4.00	K	NIST Webbook
tb	385.00 ± 3.00	K	NIST Webbook
tb	383.20	K	KDB
tb	383.45 ± 0.50	K	NIST Webbook
tb	383.50 ± 0.50	K	NIST Webbook
tb	384.00 ± 2.00	K	NIST Webbook
tb	382.30 ± 0.60	K	NIST Webbook
tb	383.45 ± 0.80	K	NIST Webbook
tb	383.50 ± 1.00	K	NIST Webbook
tb	382.00 ± 4.00	K	NIST Webbook
tb	381.00 ± 4.00	K	NIST Webbook
tb	381.90 ± 3.00	K	NIST Webbook
tb	383.40 ± 0.60	K	NIST Webbook
tb	383.47 ± 0.30	K	NIST Webbook
tb	383.50	K	NIST Webbook
tb	382.00 ± 1.00	K	NIST Webbook
tb	381.00 ± 2.00	K	NIST Webbook
tc	584.20	K	KDB
tf	152.15 ± 1.00	K	NIST Webbook
tf	152.20 ± 0.50	K	NIST Webbook
tf	152.70 ± 0.05	K	NIST Webbook
tf	152.75 ± 0.03	K	NIST Webbook
tf	152.71 ± 0.04	K	NIST Webbook
tf	152.87	K	Aqueous Solubility Prediction Method
tf	152.20	K	KDB
vc	0.354	m3/kmol	KDB
zc	0.2598130		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.22	J/mol×K	560.42	Joback Method
cpg	189.93	J/mol×K	456.92	Joback Method
cpg	176.48	J/mol×K	422.42	Joback Method
cpg	162.31	J/mol×K	387.92	Joback Method
cpg	202.69	J/mol×K	491.42	Joback Method

cpg	237.03	J/mol×K	594.92	Joback Method
cpg	214.78	J/mol×K	525.92	Joback Method
dvisc	0.0057112	Pa×s	193.55	Joback Method
dvisc	0.0002593	Pa×s	387.92	Joback Method
dvisc	0.0003433	Pa×s	355.52	Joback Method
dvisc	0.0004807	Pa×s	323.13	Joback Method
dvisc	0.0007258	Pa×s	290.74	Joback Method
dvisc	0.0012149	Pa×s	258.34	Joback Method
dvisc	0.0023575	Pa×s	225.94	Joback Method
hvapt	35.70	kJ/mol	358.50	NIST Webbook
hvapt	37.70 ± 0.20	kJ/mol	294.00	NIST Webbook
hvapt	36.70	kJ/mol	346.50	NIST Webbook
rhol	807.84	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40387e+01
Coeff. B	-3.08782e+03
Coeff. C	-5.42180e+01
Temperature range (K), min.	278.77
Temperature range (K), max.	408.03

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.21289e+01
Coeff. B	-7.17350e+03
Coeff. C	-1.00656e+01
Coeff. D	7.33952e-06
Temperature range (K), min.	333.15
Temperature range (K), max.	384.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591491&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=629
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol629.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
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
zc:	Critical Compressibility

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