Cyclohexane, chloro-

Other names:	Chlorocyclohexane
	Cyclohexyl chloride
	Monochlorocyclohexane
Inchi:	InChI=1S/C6H11Cl/c7-6-4-2-1-3-5-6/h6H,1-5H2
InchiKey:	UNFUYWDGSFDHCW-UHFFFAOYSA-N
Formula:	C6H11Cl
SMILES:	ClC1CCCCC1
Mol. weight [g/mol]:	118.61
CAS:	542-18-7

Physical Properties

Property code	Value	Unit	Source
chl	-3747.60 ± 1.90	kJ/mol	NIST Webbook
gf	12.16	kJ/mol	Joback Method
hf	-166.50 ± 1.90	kJ/mol	NIST Webbook
hf	-164.00 ± 3.00	kJ/mol	NIST Webbook
hf	-163.98 ± 0.62	kJ/mol	NIST Webbook
hfl	-206.90 ± 2.10	kJ/mol	NIST Webbook
hfl	-207.00	kJ/mol	NIST Webbook
hfl	-209.10 ± 1.90	kJ/mol	NIST Webbook
hfus	7.33	kJ/mol	Joback Method
hvap	42.92 ± 0.62	kJ/mol	NIST Webbook
hvap	42.66 ± 0.03	kJ/mol	NIST Webbook
hvap	44.00 ± 3.00	kJ/mol	NIST Webbook
hvap	40.70 ± 0.10	kJ/mol	NIST Webbook
hvap	42.90 ± 0.60	kJ/mol	NIST Webbook
hvap	41.80	kJ/mol	NIST Webbook
ie	10.10 ± 0.01	eV	NIST Webbook
ie	10.67	eV	NIST Webbook
log10ws	-2.49		Crippen Method
logp	2.558		Crippen Method
mcvol	96.780	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	870.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	874.00		NIST Webbook

rinpol	922.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	918.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1163.00		NIST Webbook
tb	393.66	K	Joback Method
tc	606.69	K	Joback Method
tf	230.15 ± 0.30	K	NIST Webbook
tf	226.00 ± 3.00	K	NIST Webbook
tf	228.80 ± 0.30	K	NIST Webbook
tf	230.00 ± 1.50	K	NIST Webbook
tf	230.10 ± 0.30	K	NIST Webbook
tt	229.34 ± 0.01	K	NIST Webbook
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.32	J/mol×K	535.68	Joback Method
cpg	239.93	J/mol×K	606.69	Joback Method
cpg	228.97	J/mol×K	571.18	Joback Method
cpg	163.54	J/mol×K	393.66	Joback Method
cpg	178.11	J/mol×K	429.16	Joback Method
cpg	191.92	J/mol×K	464.67	Joback Method
cpg	204.98	J/mol×K	500.17	Joback Method
dvisc	0.0006101	Pa×s	327.33	Joback Method
dvisc	0.0004390	Pa×s	360.50	Joback Method

dvisc	0.0003339	Pa×s	393.66	Joback Method
dvisc	0.0069833	Pa×s	194.68	Joback Method
dvisc	0.0029096	Pa×s	227.84	Joback Method
dvisc	0.0015144	Pa×s	261.01	Joback Method
dvisc	0.0009132	Pa×s	294.17	Joback Method
hfust	8.01	kJ/mol	220.40	NIST Webbook
hfust	2.04	kJ/mol	229.30	NIST Webbook
hfust	2.04	kJ/mol	154.50	NIST Webbook
hfust	1.67	kJ/mol	228.70	NIST Webbook
hfust	0.05	kJ/mol	120.00	NIST Webbook
hvapt	39.30	kJ/mol	383.00	NIST Webbook
rhol	993.17	kg/m3	298.15	Study of the Surface Tension of Chlorocyclohexane or Bromocyclohexane with Some Cyclic Ethers
sfust	8.91	J/mol×K	229.30	NIST Webbook
sfust	36.35	J/mol×K	220.40	NIST Webbook
sfust	0.42	J/mol×K	120.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73833e+01
Coeff. B	-4.28877e+03
Coeff. C	-5.20550e+01
Temperature range (K), min.	302.92
Temperature range (K), max.	407.33

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C542187&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
Study of the Surface Tension of Chlorocyclohexane or Bromocyclohexane with Some Cyclic Ethers:	https://www.doi.org/10.1021/je0500577

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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume