Cyclohexene, 4-methyl-

Other names:	4-METHYL-1-CYCLOHEXENE
	4-METHYLCYCLOHEXENE
	4-Methylcyclohex-1-ene
	4-Methylcyclohexene-1
Inchi:	InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h2-3,7H,4-6H2,1H3
InchiKey:	FSWCCQWDVGZMRD-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC1CC=CCC1
Mol. weight [g/mol]:	96.17
CAS:	591-47-9

Physical Properties

Property code	Value	Unit	Source
chl	-4395.00 ± 4.00	kJ/mol	NIST Webbook
gf	62.47	kJ/mol	Joback Method
hf	-75.71	kJ/mol	Joback Method
hfl	-75.00 ± 4.00	kJ/mol	NIST Webbook
hfus	6.94	kJ/mol	Joback Method
hvap	36.30 ± 0.60	kJ/mol	NIST Webbook
ie	8.92	eV	NIST Webbook
ie	8.91 ± 0.01	eV	NIST Webbook
ie	8.91 ± 0.01	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	2.363		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
rinpol	733.20		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	739.50		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	739.10		NIST Webbook
rinpol	747.10		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	751.20		NIST Webbook
rinpol	95.60		NIST Webbook
rinpol	748.00		NIST Webbook

rinpol	744.00	NIST Webbook
rinpol	744.60	NIST Webbook
rinpol	739.90	NIST Webbook
rinpol	757.50	NIST Webbook
rinpol	95.60	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	733.00	NIST Webbook
rinpol	733.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	742.80	NIST Webbook
rinpol	739.50	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	738.00	NIST Webbook
rinpol	738.10	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	746.00	NIST Webbook
rinpol	739.10	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	745.50	NIST Webbook
rinpol	747.10	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	747.10	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	729.60	NIST Webbook
rinpol	736.30	NIST Webbook
rinpol	741.80	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	738.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	729.80	NIST Webbook
rinpol	729.83	NIST Webbook

rinpol	730.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	751.20		NIST Webbook
rinpol	748.00		NIST Webbook
ripol	893.10		NIST Webbook
ripol	884.00		NIST Webbook
ripol	859.00		NIST Webbook
ripol	859.00		NIST Webbook
ripol	849.00		NIST Webbook
ripol	883.90		NIST Webbook
ripol	874.00		NIST Webbook
ripol	849.00		NIST Webbook
ripol	883.90		NIST Webbook
ripol	874.00		NIST Webbook
ripol	893.10		NIST Webbook
ripol	893.00		NIST Webbook
ripol	869.00		NIST Webbook
ripol	893.00		NIST Webbook
ripol	883.00		NIST Webbook
ripol	874.00		NIST Webbook
sl	253.01	J/mol×K	NIST Webbook
tb	377.00 ± 5.00	K	NIST Webbook
tb	375.92 ± 0.40	K	NIST Webbook
tb	375.89 ± 0.20	K	NIST Webbook
tb	375.00 ± 2.00	K	NIST Webbook
tb	375.88 ± 0.30	K	NIST Webbook
tb	376.30 ± 0.50	K	NIST Webbook
tb	375.70 ± 5.00	K	NIST Webbook
tb	376.00 ± 0.10	K	NIST Webbook
tb	374.70	K	NIST Webbook
tc	582.97	K	Joback Method
tf	156.88 ± 0.60	K	NIST Webbook
tf	157.40 ± 0.30	K	NIST Webbook
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.15	J/mol×K	548.85	Joback Method
cpg	203.22	J/mol×K	480.62	Joback Method
cpg	189.70	J/mol×K	446.50	Joback Method
cpg	175.47	J/mol×K	412.39	Joback Method
cpg	160.50	J/mol×K	378.27	Joback Method
cpg	216.03	J/mol×K	514.73	Joback Method
cpg	239.62	J/mol×K	582.97	Joback Method
cpl	180.42	J/mol×K	298.15	NIST Webbook
dvisc	0.0052144	Pa×s	176.79	Joback Method
dvisc	0.0002578	Pa×s	378.27	Joback Method
dvisc	0.0003334	Pa×s	344.69	Joback Method
dvisc	0.0004557	Pa×s	311.11	Joback Method
dvisc	0.0006718	Pa×s	277.53	Joback Method
dvisc	0.0011021	Pa×s	243.95	Joback Method
dvisc	0.0021175	Pa×s	210.37	Joback Method
hfust	6.63	kJ/mol	153.60	NIST Webbook
hfust	6.63	kJ/mol	153.60	NIST Webbook
hvapt	36.30	kJ/mol	360.50	NIST Webbook
hvapt	37.00 ± 0.60	kJ/mol	285.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39002e+01
Coeff. B	-2.99749e+03
Coeff. C	-5.30590e+01
Temperature range (K), min.	273.26
Temperature range (K), max.	402.06

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.94074e+01
Coeff. B	-6.91563e+03
Coeff. C	-9.67948e+00
Coeff. D	7.08774e-06
Temperature range (K), min.	292.15
Temperature range (K), max.	429.15

Sources

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=631
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=631
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591479&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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