Cyclohexene, 3-methyl-

Other names:	3-METHYL-1-CYCLOHEXENE
	3-METHYLCYCLOHEXENE
	3-Methylcyclohex-1-ene
	3-Methylcyclohexene-1
Inchi:	InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h3,5,7H,2,4,6H2,1H3
InchiKey:	UZPWKTCMUADILM-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC1C=CCCC1
Mol. weight [g/mol]:	96.17
CAS:	591-48-0

Physical Properties

Property code	Value	Unit	Source
gf	62.47	kJ/mol	Joback Method
hf	-75.71	kJ/mol	Joback Method
hfus	6.94	kJ/mol	Joback Method
hvap	31.90	kJ/mol	Joback Method
ie	8.89 ± 0.01	eV	NIST Webbook
ie	9.12	eV	NIST Webbook
ie	8.94 ± 0.03	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	747.00		NIST Webbook
rinpol	755.80		NIST Webbook
rinpol	749.70		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	743.30		NIST Webbook
rinpol	735.70		NIST Webbook

rinpol	762.00	NIST Webbook
rinpol	730.60	NIST Webbook
rinpol	735.70	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	735.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	735.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	745.50	NIST Webbook
rinpol	745.50	NIST Webbook
rinpol	745.50	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	727.10	NIST Webbook
rinpol	733.70	NIST Webbook
rinpol	738.80	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	729.06	NIST Webbook
rinpol	729.10	NIST Webbook
rinpol	729.00	NIST Webbook
rinpol	745.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	742.90	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	729.06	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	740.00	NIST Webbook

rinpol	737.70		NIST Webbook
ripol	870.00		NIST Webbook
ripol	873.00		NIST Webbook
ripol	888.00		NIST Webbook
ripol	888.00		NIST Webbook
ripol	887.90		NIST Webbook
ripol	870.00		NIST Webbook
ripol	879.20		NIST Webbook
ripol	887.90		NIST Webbook
ripol	870.00		NIST Webbook
ripol	879.20		NIST Webbook
ripol	847.00		NIST Webbook
ripol	852.00		NIST Webbook
ripol	847.00		NIST Webbook
ripol	888.00		NIST Webbook
ripol	870.00		NIST Webbook
ripol	879.00		NIST Webbook
ripol	866.00		NIST Webbook
tb	378.27	K	Joback Method
tc	582.97	K	Joback Method
tf	152.15 ± 0.50	K	NIST Webbook
tf	150.05 ± 0.10	K	NIST Webbook
tf	149.70 ± 1.00	K	NIST Webbook
tf	150.30 ± 2.00	K	NIST Webbook
tf	147.30 ± 2.00	K	NIST Webbook
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.62	J/mol×K	582.97	Joback Method
cpg	228.15	J/mol×K	548.85	Joback Method
cpg	216.03	J/mol×K	514.73	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
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
hvapt	34.80	kJ/mol	355.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37765e+01
Coeff. B	-2.96157e+03
Coeff. C	-5.36190e+01
Temperature range (K), min.	273.18
Temperature range (K), max.	403.48

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591480&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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=630

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

Legend

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
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