Cyclohexane, 1,3-dimethyl-, cis-

Other names:	1,3-Dimethylcyclohexane, cis- 1,3-dimethyl(cis)-cyclohexane 1,CIS-3-DIMETHYLCYCLOHEXANE CIS-1,3-DIMETHYLCYCLOHEXANE Cyclohexane, cis-1,3-dimethyl- NSC 74159 c-1,3-Dimethylcyclohexane
Inchi:	InChI=1S/C8H16/c1-7-4-3-5-8(2)6-7/h7-8H,3-6H2,1-2H3/t7-,8+
InchiKey:	SGVUHPSBDNVHKL-OCAPTIKFSA-N
Formula:	C8H16
SMILES:	CC1CCCC(C)C1
Mol. weight [g/mol]:	112.21
CAS:	638-04-0

Physical Properties

Property code	Value	Unit	Source
af	0.2240		KDB
ap	324.850	K	KDB
chl	-5211.80 ± 1.70	kJ/mol	NIST Webbook
gf	29.85	kJ/mol	KDB
hcg	5211.80	kJ/mol	KDB
hcn	4859.716	kJ/mol	KDB
hf	-184.90	kJ/mol	KDB
hfus	9.38	kJ/mol	Joback Method
hvap	38.22	kJ/mol	NIST Webbook
hvap	38.20 ± 0.10	kJ/mol	NIST Webbook
hvap	38.20	kJ/mol	NIST Webbook
hvap	38.10	kJ/mol	NIST Webbook
hvap	38.31	kJ/mol	NIST Webbook
ie	9.98 ± 0.05	eV	NIST Webbook
log10ws	-2.58		Crippen Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2900.00	kPa	KDB
rinpol	789.80		NIST Webbook
rinpol	784.70		NIST Webbook
rinpol	789.60		NIST Webbook

rinpol	773.30	NIST Webbook
rinpol	775.50	NIST Webbook
rinpol	777.90	NIST Webbook
rinpol	780.20	NIST Webbook
rinpol	785.10	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	778.40	NIST Webbook
rinpol	778.60	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	784.90	NIST Webbook
rinpol	784.70	NIST Webbook
rinpol	789.70	NIST Webbook
rinpol	790.10	NIST Webbook
rinpol	790.80	NIST Webbook
rinpol	790.80	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	769.80	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	776.60	NIST Webbook
rinpol	772.80	NIST Webbook
rinpol	774.70	NIST Webbook
rinpol	776.60	NIST Webbook
rinpol	783.30	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	772.80	NIST Webbook
rinpol	774.70	NIST Webbook

rinpol	776.60	NIST Webbook
rinpol	770.23	NIST Webbook
rinpol	771.54	NIST Webbook
rinpol	771.77	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	767.70	NIST Webbook
rinpol	770.50	NIST Webbook
rinpol	772.28	NIST Webbook
rinpol	771.53	NIST Webbook
rinpol	774.44	NIST Webbook
rinpol	776.29	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	785.32	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	784.40	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	788.50	NIST Webbook
rinpol	790.50	NIST Webbook
rinpol	792.20	NIST Webbook
rinpol	793.70	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	785.32	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	769.80	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	780.30	NIST Webbook
rinpol	774.90	NIST Webbook
rinpol	778.10	NIST Webbook
rinpol	778.60	NIST Webbook
rinpol	778.50	NIST Webbook
rinpol	778.40	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	770.00	NIST Webbook

rinpol	789.70		NIST Webbook
ripol	810.00		NIST Webbook
ripol	810.00		NIST Webbook
sg	371.20	J/mol×K	NIST Webbook
sl	272.63	J/mol×K	NIST Webbook
tb	398.10 ± 2.00	K	NIST Webbook
tb	394.70 ± 2.00	K	NIST Webbook
tb	393.55 ± 0.30	K	NIST Webbook
tb	393.30	K	KDB
tb	393.20	K	NIST Webbook
tb	393.30	K	NIST Webbook
tb	393.50 ± 0.30	K	NIST Webbook
tb	393.70 ± 0.50	K	NIST Webbook
tb	393.00 ± 2.00	K	NIST Webbook
tb	393.56 ± 0.30	K	NIST Webbook
tb	393.20 ± 1.00	K	NIST Webbook
tb	392.15 ± 0.50	K	NIST Webbook
tb	393.65 ± 0.50	K	NIST Webbook
tb	393.85 ± 0.60	K	NIST Webbook
tb	393.15 ± 0.10	K	NIST Webbook
tb	394.15 ± 0.60	K	NIST Webbook
tb	393.75 ± 0.50	K	NIST Webbook
tb	393.15 ± 0.70	K	NIST Webbook
tb	393.45 ± 0.30	K	NIST Webbook
tb	393.24 ± 0.20	K	NIST Webbook
tb	397.85 ± 0.30	K	NIST Webbook
tb	392.65 ± 0.50	K	NIST Webbook
tb	392.70 ± 2.00	K	NIST Webbook
tb	392.65 ± 0.50	K	NIST Webbook
tb	393.23 ± 0.02	K	NIST Webbook
tc	591.00	K	KDB
tc	591.00	K	NIST Webbook
tf	177.95 ± 0.20	K	NIST Webbook
tf	197.60	K	KDB
tf	194.15 ± 3.00	K	NIST Webbook
tf	196.09 ± 0.02	K	NIST Webbook
tt	197.59 ± 0.03	K	NIST Webbook
tt	197.59 ± 0.02	K	NIST Webbook
tt	197.58 ± 0.05	K	NIST Webbook
vc	0.449	m3/kmol	KDB
zc	0.2649250		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.84	J/mol×K	530.89	Joback Method
cpg	263.41	J/mol×K	497.49	Joback Method
cpg	307.47	J/mol×K	597.67	Joback Method
cpg	293.52	J/mol×K	564.28	Joback Method
cpg	212.54	J/mol×K	397.32	Joback Method
cpg	230.28	J/mol×K	430.71	Joback Method
cpg	247.23	J/mol×K	464.10	Joback Method
cpl	209.37	J/mol×K	298.15	NIST Webbook
dvisc	0.0041986	Pa×s	183.06	Joback Method
dvisc	0.0018154	Pa×s	218.77	Joback Method
dvisc	0.0009932	Pa×s	254.48	Joback Method
dvisc	0.0006303	Pa×s	290.19	Joback Method
dvisc	0.0002631	Pa×s	397.32	Joback Method
dvisc	0.0003324	Pa×s	361.61	Joback Method
dvisc	0.0004419	Pa×s	325.90	Joback Method
hfust	10.82	kJ/mol	197.60	NIST Webbook
hfust	10.82	kJ/mol	197.60	NIST Webbook
hfust	10.82	kJ/mol	197.59	NIST Webbook
hvapt	37.70	kJ/mol	357.00	NIST Webbook
hvapt	32.80	kJ/mol	393.30	KDB
hvapt	32.91	kJ/mol	393.30	NIST Webbook
hvapt	36.80	kJ/mol	357.00	NIST Webbook
hvapt	34.90 ± 0.10	kJ/mol	363.00	NIST Webbook
hvapt	33.30 ± 0.10	kJ/mol	385.00	NIST Webbook
rfi	1.42063		298.15	KDB
rhol	766.00	kg/m3	293.00	KDB
sfust	54.77	J/mol×K	197.59	NIST Webbook
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38755e+01
Coeff. B	-3.19163e+03

Coeff. C	-4.82270e+01
Temperature range (K), min.	283.11
Temperature range (K), max.	420.90

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.27551e+01
Coeff. B	-6.92278e+03
Coeff. C	-8.58765e+00
Coeff. D	5.00269e-06
Temperature range (K), min.	197.58
Temperature range (K), max.	591.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=499

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=499

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C638040&Units=SI

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

Legend

af: Acentric Factor

ap: Aniline Point

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

hcg: Heat of Combustion, Gross form

hcn: Heat of Combustion, Net Form

hf: 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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility