Cyclohexane, 1,1-dimethyl-

Other names: 1,1-Dimethylcyclohexane
GEM-DIMETHYLCYCLOHEXANE
Inchi: InChI=1S/C8H16/c1-8(2)6-4-3-5-7-8/h3-7H2,1-2H3
InchiKey: QEGNUYASOUJEHD-UHFFFAOYSA-N
Formula: C8H16
SMILES: CC1(C)CCCCC1
Mol. weight [g/mol]: 112.21
CAS: 590-66-9

Physical Properties

Property code	Value	Unit	Source
af	0.2380		KDB
ap	318.550	K	KDB
chl	-5241.30	kJ/mol	NIST Webbook
chl	-5216.00 ± 1.90	kJ/mol	NIST Webbook
gf	35.25	kJ/mol	KDB
hcg	5215.98	kJ/mol	KDB
hcn	4863.900	kJ/mol	KDB
hf	-181.10	kJ/mol	KDB
hfus	2.01	kJ/mol	Joback Method
hvap	38.80 ± 0.10	kJ/mol	NIST Webbook
hvap	37.80	kJ/mol	NIST Webbook
hvap	37.90	kJ/mol	NIST Webbook
hvap	37.97	kJ/mol	NIST Webbook
ie	9.42	eV	NIST Webbook
ie	9.50 ± 0.05	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.977		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2960.00	kPa	KDB
rinpol	784.00		NIST Webbook
rinpol	789.80		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	786.40		NIST Webbook
rinpol	786.90		NIST Webbook
rinpol	792.00		NIST Webbook

rinpol	779.80	NIST Webbook
rinpol	782.60	NIST Webbook
rinpol	785.40	NIST Webbook
rinpol	788.50	NIST Webbook
rinpol	787.10	NIST Webbook
rinpol	786.10	NIST Webbook
rinpol	786.50	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	797.60	NIST Webbook
rinpol	797.70	NIST Webbook
rinpol	791.30	NIST Webbook
rinpol	792.70	NIST Webbook
rinpol	787.00	NIST Webbook
rinpol	793.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	791.12	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	780.30	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	784.20	NIST Webbook
rinpol	778.31	NIST Webbook
rinpol	782.50	NIST Webbook
rinpol	779.57	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	791.12	NIST Webbook
rinpol	787.00	NIST Webbook
rinpol	797.00	NIST Webbook
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rinpol	793.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	784.00		NIST Webbook
sg	364.93	J/mol×K	NIST Webbook
sl	267.23	J/mol×K	NIST Webbook
tb	392.70	K	KDB
tc	591.00	K	KDB
tf	239.70	K	KDB
tf	239.13 ± 0.20	K	NIST Webbook
tf	239.61 ± 0.07	K	NIST Webbook
tf	237.95 ± 0.50	K	NIST Webbook
tt	239.81 ± 0.05	K	NIST Webbook
tt	239.81 ± 0.05	K	NIST Webbook
vc	0.416	m3/kmol	KDB
zc	0.2505880		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.90	J/mol×K	507.35	Joback Method
cpg	306.89	J/mol×K	612.48	Joback Method
cpg	293.78	J/mol×K	577.44	Joback Method
cpg	279.81	J/mol×K	542.39	Joback Method
cpg	213.43	J/mol×K	402.23	Joback Method
cpg	231.81	J/mol×K	437.27	Joback Method
cpg	248.93	J/mol×K	472.31	Joback Method
cpl	209.24	J/mol×K	298.15	NIST Webbook
hfust	2.01	kJ/mol	239.80	NIST Webbook

hfust	5.98	kJ/mol	153.20	NIST Webbook
hfust	2.01	kJ/mol	239.80	NIST Webbook
hvapt	36.60	kJ/mol	354.00	NIST Webbook
hvapt	32.59	kJ/mol	392.70	KDB
hvapt	32.51	kJ/mol	392.70	NIST Webbook
hvapt	39.60 ± 0.10	kJ/mol	287.00	NIST Webbook
rfi	1.42662		298.15	KDB
rhol	785.00	kg/m3	289.00	KDB
sfust	8.37	J/mol×K	239.80	NIST Webbook
sfust	39.05	J/mol×K	153.20	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	1.37664e+01
Coeff. B	-3.13309e+03
Coeff. C	-5.05140e+01
Temperature range (K), min.	282.96
Temperature range (K), max.	421.08

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.41338e+01
Coeff. B	-6.91909e+03
Coeff. C	-8.82986e+00
Coeff. D	5.47352e-06
Temperature range (K), min.	239.66
Temperature range (K), max.	591.15

Sources

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/files/research/kdb/mol/mol496.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590669&Units=SI
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=496

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
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