Cyclohexane, 1,4-dimethyl-, cis-

Other names:	1,4(cis)-dimethylcyclohexane
	1,4-Dimethylcyclohexane, cis-
	1,CIS-4-DIMETHYLCYCLOHEXANE
	CIS-1,4-DIMETHYLCYCLOHEXANE
	Cyclohexane, cis-1,4-dimethyl-
Inchi:	InChI=1S/C8H16/c1-7-3-5-8(2)6-4-7/h7-8H,3-6H2,1-2H3/t7-,8+
InchiKey:	QRMPKOFEUHIBNM-OCAPTIKFSA-N
Formula:	C8H16
SMILES:	CC1CCC(C)CC1
Mol. weight [g/mol]:	112.21
CAS:	624-29-3

Physical Properties

Property code	Value	Unit	Source
af	0.2340		KDB
ap	320.050	K	KDB
chl	-5219.10 ± 1.70	kJ/mol	NIST Webbook
gf	37.97	kJ/mol	KDB
hcg	5219.12	kJ/mol	KDB
hcn	4867.038	kJ/mol	KDB
hf	-176.80	kJ/mol	KDB
hfus	9.38	kJ/mol	Joback Method
hvap	3900.00	kJ/mol	NIST Webbook
hvap	39.00	kJ/mol	NIST Webbook
hvap	39.00 ± 0.10	kJ/mol	NIST Webbook
hvap	39.02	kJ/mol	NIST Webbook
hvap	39.07	kJ/mol	NIST Webbook
ie	9.93 ± 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	813.10		NIST Webbook
rinpol	838.20		NIST Webbook
rinpol	804.60		NIST Webbook
rinpol	804.50		NIST Webbook
rinpol	815.30		NIST Webbook

rinpol	816.00	NIST Webbook
rinpol	814.30	NIST Webbook
rinpol	822.00	NIST Webbook
rinpol	812.40	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	802.80	NIST Webbook
rinpol	805.70	NIST Webbook
rinpol	838.20	NIST Webbook
rinpol	823.40	NIST Webbook
rinpol	828.30	NIST Webbook
rinpol	837.40	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	804.60	NIST Webbook
rinpol	804.60	NIST Webbook
rinpol	809.80	NIST Webbook
rinpol	805.00	NIST Webbook
rinpol	804.10	NIST Webbook
rinpol	804.50	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	809.60	NIST Webbook
rinpol	811.90	NIST Webbook
rinpol	815.10	NIST Webbook
rinpol	815.30	NIST Webbook
rinpol	810.70	NIST Webbook
rinpol	810.80	NIST Webbook
rinpol	813.10	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	822.00	NIST Webbook
rinpol	829.00	NIST Webbook
rinpol	833.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	805.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	805.50	NIST Webbook
rinpol	801.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	801.20	NIST Webbook
rinpol	802.80	NIST Webbook
rinpol	772.45	NIST Webbook
rinpol	770.01	NIST Webbook

rinpol	804.70		NIST Webbook
rinpol	805.30		NIST Webbook
rinpol	805.70		NIST Webbook
rinpol	802.20		NIST Webbook
rinpol	804.70		NIST Webbook
rinpol	805.30		NIST Webbook
rinpol	805.70		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	805.20		NIST Webbook
rinpol	807.20		NIST Webbook
rinpol	810.10		NIST Webbook
rinpol	761.00		NIST Webbook
sg	370.87	J/mol×K	NIST Webbook
sl	271.12	J/mol×K	NIST Webbook
tb	397.60	K	KDB
tc	598.00	K	KDB
tf	186.45 ± 0.70	K	NIST Webbook
tf	185.42 ± 0.02	K	NIST Webbook
tf	185.72 ± 0.03	K	NIST Webbook
tf	186.50 ± 0.50	K	NIST Webbook
tf	185.70	K	KDB
tf	185.46 ± 0.20	K	NIST Webbook
tt	185.73 ± 0.02	K	NIST Webbook
tt	185.72 ± 0.05	K	NIST Webbook
tt	195.73 ± 0.02	K	NIST Webbook
vc	0.471	m3/kmol	KDB
zc	0.2748890		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.23	J/mol×K	464.10	Joback Method
cpg	307.47	J/mol×K	597.67	Joback Method
cpg	293.52	J/mol×K	564.28	Joback Method
cpg	278.84	J/mol×K	530.89	Joback Method
cpg	263.41	J/mol×K	497.49	Joback Method
cpg	212.54	J/mol×K	397.32	Joback Method

cpg	230.28	J/mol×K	430.71	Joback Method
cpl	212.09	J/mol×K	298.15	NIST Webbook
dvisc	0.0041986	Pa×s	183.06	Joback Method
dvisc	0.0009932	Pa×s	254.48	Joback Method
dvisc	0.0006303	Pa×s	290.19	Joback Method
dvisc	0.0004419	Pa×s	325.90	Joback Method
dvisc	0.0003324	Pa×s	361.61	Joback Method
dvisc	0.0018154	Pa×s	218.77	Joback Method
dvisc	0.0002631	Pa×s	397.32	Joback Method
hfust	9.29	kJ/mol	185.70	NIST Webbook
hfust	9.31	kJ/mol	185.73	NIST Webbook
hfust	9.31	kJ/mol	185.70	NIST Webbook
hvapt	33.28	kJ/mol	397.50	NIST Webbook
hvapt	33.77	kJ/mol	397.60	KDB
hvapt	37.60	kJ/mol	358.50	NIST Webbook
rfi	1.42731		298.15	KDB
rhol	783.00	kg/m3	293.00	KDB
sfust	50.11	J/mol×K	185.73	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	1.38911e+01
Coeff. B	-3.23780e+03
Coeff. C	-4.78270e+01
Temperature range (K), min.	285.84
Temperature range (K), max.	425.21

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.15606e+01
Coeff. B	-6.96889e+03
Coeff. C	-8.37542e+00
Coeff. D	4.54960e-06
Temperature range (K), min.	185.72
Temperature range (K), max.	598.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624293&Units=SI
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=501
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=501
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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