Cyclohexane, 1,4-dimethyl-, trans-

Other names:	1,4(trans)-dimethylcyclohexane 1,4-Dimethylcyclohexane, trans- 1,TRANS-4-DIMETHYLCYCLOHEXANE Cyclohexane, trans-1,4-dimethyl- TRANS-1,4-DIMETHYLCYCLOHEXANE t-1,4-Dimethylcyclohexane
Inchi:	InChI=1S/C8H16/c1-7-3-5-8(2)6-4-7/h7-8H,3-6H2,1-2H3/t7-,8-
InchiKey:	QRMPKOFEUHIBNM-ZKCHVHJHSA-N
Formula:	C8H16
SMILES:	CC1CCC(C)CC1
Mol. weight [g/mol]:	112.21
CAS:	2207-04-7

Physical Properties

Property code	Value	Unit	Source
af	0.2420		KDB
ap	325.850	K	KDB
chl	-5212.30 ± 1.70	kJ/mol	NIST Webbook
gf	31.74	kJ/mol	KDB
hcg	5212.34	kJ/mol	KDB
hcn	4860.260	kJ/mol	KDB
hf	-184.70	kJ/mol	KDB
hfus	9.38	kJ/mol	Joback Method
hvap	37.87	kJ/mol	NIST Webbook
hvap	39.90 ± 0.10	kJ/mol	NIST Webbook
hvap	37.60	kJ/mol	NIST Webbook
hvap	37.95	kJ/mol	NIST Webbook
hvap	37.90	kJ/mol	NIST Webbook
ie	9.56	eV	NIST Webbook
ie	9.92 ± 0.05	eV	NIST Webbook
log10ws	-4.47		Estimated Solubility Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2970.00	kPa	KDB
rinpol	796.00		NIST Webbook
rinpol	779.60		NIST Webbook

rinpol	782.00	NIST Webbook
rinpol	785.60	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	780.20	NIST Webbook
rinpol	780.50	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	784.10	NIST Webbook
rinpol	791.90	NIST Webbook
rinpol	790.20	NIST Webbook
rinpol	790.80	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	777.20	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	774.50	NIST Webbook
rinpol	778.50	NIST Webbook
rinpol	772.09	NIST Webbook
rinpol	770.39	NIST Webbook
rinpol	774.90	NIST Webbook
rinpol	776.70	NIST Webbook
rinpol	777.30	NIST Webbook
rinpol	785.40	NIST Webbook
rinpol	776.70	NIST Webbook
rinpol	775.60	NIST Webbook
rinpol	776.70	NIST Webbook
rinpol	777.30	NIST Webbook

rinpol	774.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	784.60		NIST Webbook
rinpol	786.10		NIST Webbook
rinpol	788.40		NIST Webbook
rinpol	790.20		NIST Webbook
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rinpol	793.10		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	790.30		NIST Webbook
rinpol	786.20		NIST Webbook
rinpol	784.90		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	779.90		NIST Webbook
rinpol	780.50		NIST Webbook
rinpol	780.30		NIST Webbook
rinpol	780.20		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	802.60		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	816.70		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	775.60		NIST Webbook
rinpol	788.00		NIST Webbook
sg	365.89	J/mol×K	NIST Webbook
sl	268.03	J/mol×K	NIST Webbook
tb	392.50	K	KDB
tc	5877.70 ± 0.50	K	NIST Webbook
tc	587.70 ± 0.58	K	NIST Webbook
tc	590.00	K	NIST Webbook

tc	587.70	K	KDB
tf	236.20	K	KDB
tt	236.22 ± 0.02	K	NIST Webbook
vc	0.450	m3/kmol	KDB
zc	0.2735120		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	247.23	J/mol×K	464.10	Joback Method
cpg	230.28	J/mol×K	430.71	Joback Method
cpg	212.54	J/mol×K	397.32	Joback Method
cpl	210.25	J/mol×K	298.15	NIST Webbook
dvisc	0.0004419	Pa×s	325.90	Joback Method
dvisc	0.0002631	Pa×s	397.32	Joback Method
dvisc	0.0006303	Pa×s	290.19	Joback Method
dvisc	0.0009932	Pa×s	254.48	Joback Method
dvisc	0.0018154	Pa×s	218.77	Joback Method
dvisc	0.0041986	Pa×s	183.06	Joback Method
dvisc	0.0003324	Pa×s	361.61	Joback Method
hfust	12.34	kJ/mol	236.20	NIST Webbook
hfust	12.34	kJ/mol	236.20	NIST Webbook
hfust	12.33	kJ/mol	236.22	NIST Webbook
hvapt	32.59	kJ/mol	392.50	KDB
hvapt	32.56	kJ/mol	392.50	NIST Webbook
hvapt	36.70	kJ/mol	354.00	NIST Webbook
hvapt	35.60 ± 0.10	kJ/mol	341.00	NIST Webbook
hvapt	34.60 ± 0.10	kJ/mol	357.00	NIST Webbook
hvapt	33.50 ± 0.10	kJ/mol	377.00	NIST Webbook
rfi	1.41853		298.15	KDB
rhol	763.00	kg/m3	293.00	KDB
sfust	52.21	J/mol×K	236.22	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	1.38145e+01
Coeff. B	-3.15127e+03
Coeff. C	-4.99260e+01
Temperature range (K), min.	282.89
Temperature range (K), max.	420.53

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.42070e+01
Coeff. B	-6.91805e+03
Coeff. C	-8.84557e+00
Coeff. D	5.63363e-06
Temperature range (K), min.	236.21
Temperature range (K), max.	590.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=502
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=502
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2207047&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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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