Cyclohexane, 1,3-dimethyl-, trans-

Other names:	1,3(trans)-dimethylcyclohexane
	1,3-Dimethyl(trans)-cyclohexane
	1,3-Dimethylcyclohexane, trans
	1,TRANS-3-DIMETHYLCYCLOHEXANE
	Cyclohexane, trans-1,3-dimethyl-
	TRANS-1,3-DIMETHYLCYCLOHEXANE
Inchi:	InChI=1S/C8H16/c1-7-4-3-5-8(2)6-7/h7-8H,3-6H2,1-2H3/t7-,8-/m0/s1
InchiKey:	SGVUHPSBDNVHKL-YUMQZZPRSA-N
Formula:	C8H16
SMILES:	CC1CCCC(C)C1
Mol. weight [g/mol]:	112.21
CAS:	2207-03-6

Physical Properties

Property code	Value	Unit	Source
af	0.1890		KDB
ap	319.450	K	KDB
chl	-5219.00 ± 1.70	kJ/mol	NIST Webbook
gf	36.34	kJ/mol	KDB
hcg	5219.04	kJ/mol	KDB
hcn	4866.954	kJ/mol	KDB
hf	-176.70	kJ/mol	KDB
hfus	9.38	kJ/mol	Joback Method
hvap	39.20	kJ/mol	NIST Webbook
hvap	39.21	kJ/mol	NIST Webbook
hvap	39.19	kJ/mol	NIST Webbook
hvap	39.10	kJ/mol	NIST Webbook
hvap	39.20 ± 0.10	kJ/mol	NIST Webbook
ie	9.89 ± 0.05	eV	NIST Webbook
ie	9.53	eV	NIST Webbook
ie	9.52 ± 0.05	eV	NIST Webbook
ie	9.53	eV	NIST Webbook
log10ws	-2.58		Crippen Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2970.00	kPa	KDB
rinpol	807.60		NIST Webbook

rinpol	810.60	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	805.60	NIST Webbook
rinpol	814.90	NIST Webbook
rinpol	816.60	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	802.60	NIST Webbook
rinpol	810.80	NIST Webbook
rinpol	803.90	NIST Webbook
rinpol	804.10	NIST Webbook
rinpol	804.20	NIST Webbook
rinpol	804.30	NIST Webbook
rinpol	804.10	NIST Webbook
rinpol	805.60	NIST Webbook
rinpol	810.80	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	804.90	NIST Webbook
rinpol	804.60	NIST Webbook
rinpol	809.80	NIST Webbook
rinpol	805.40	NIST Webbook
rinpol	803.90	NIST Webbook
rinpol	804.30	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	805.30	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	813.10	NIST Webbook
rinpol	813.10	NIST Webbook
rinpol	822.00	NIST Webbook
rinpol	829.00	NIST Webbook
rinpol	833.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	802.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	805.50	NIST Webbook
rinpol	802.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	806.00	NIST Webbook

rinpol	810.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	808.84		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	798.70		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	802.80		NIST Webbook
rinpol	804.10		NIST Webbook
rinpol	805.30		NIST Webbook
rinpol	806.20		NIST Webbook
rinpol	802.20		NIST Webbook
rinpol	804.10		NIST Webbook
rinpol	805.30		NIST Webbook
rinpol	806.20		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	810.50		NIST Webbook
rinpol	806.00		NIST Webbook
ripol	843.00		NIST Webbook
sg	376.39	J/mol×K	NIST Webbook
sl	276.27	J/mol×K	NIST Webbook
tb	397.60	K	KDB
tc	598.00	K	KDB
tf	179.76 ± 0.02	K	NIST Webbook
tf	183.00	K	KDB
tf	406.83 ± 0.06	K	NIST Webbook
tf	196.45 ± 0.50	K	NIST Webbook
tt	183.03 ± 0.05	K	NIST Webbook
tt	183.06 ± 0.02	K	NIST Webbook
tt	183.06 ± 0.02	K	NIST Webbook
vc	0.415	m3/kmol	KDB
zc	0.2481930		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	263.41	J/mol×K	497.49	Joback Method
cpg	278.84	J/mol×K	530.89	Joback Method
cpg	293.52	J/mol×K	564.28	Joback Method

cpg	307.47	J/mol×K	597.67	Joback Method
cpl	212.84	J/mol×K	298.15	NIST Webbook
dvisc	0.0041986	Pa×s	183.06	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
dvisc	0.0004419	Pa×s	325.90	Joback Method
dvisc	0.0006303	Pa×s	290.19	Joback Method
dvisc	0.0009932	Pa×s	254.48	Joback Method
hfust	9.87	kJ/mol	183.10	NIST Webbook
hfust	9.87	kJ/mol	183.06	NIST Webbook
hfust	9.87	kJ/mol	183.10	NIST Webbook
hvapt	37.90	kJ/mol	357.00	NIST Webbook
hvapt	37.40	kJ/mol	354.00	NIST Webbook
hvapt	33.39	kJ/mol	397.60	NIST Webbook
hvapt	33.85	kJ/mol	397.60	KDB
rfi	1.42843		298.15	KDB
rhol	785.00	kg/m3	293.00	KDB
sfust	53.89	J/mol×K	183.06	NIST Webbook
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39936e+01
Coeff. B	-3.26162e+03
Coeff. C	-4.81030e+01
Temperature range (K), min.	286.07
Temperature range (K), max.	423.77

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.23828e+01
Coeff. B	-7.02468e+03
Coeff. C	-8.49035e+00
Coeff. D	4.56712e-06
Temperature range (K), min.	183.05

Temperature range (K), max.	598.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=500
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2207036&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=500
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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