Cyclohexane, (1,1-dimethylethyl)-

Other names:	(1,1-DIMETHYLETHYL)CYCLOHEXANE
	1,1-dimethylethylcyclohexane
	1-tert-Butylcyclohexane
	2-cyclohexyl-2-methylpropane
	Cyclohexane, t-butyl-
	Cyclohexane, tert-butyl-
	t-Butylcyclohexane
	tert-Butylcyclohexane
Inchi:	InChI=1S/C10H20/c1-10(2,3)9-7-5-4-6-8-9/h9H,4-8H2,1-3H3
InchiKey:	XTVMZZBLCLWBPM-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	CC(C)(C)C1CCCCC1
Mol. weight [g/mol]:	140.27
CAS:	3178-22-1

Physical Properties

Property code	Value	Unit	Source
af	0.2520		KDB
dm	0.00	debye	KDB
gf	60.61	kJ/mol	Joback Method
hf	-204.16	kJ/mol	Joback Method
hfus	6.08	kJ/mol	Joback Method
hvap	46.98	kJ/mol	NIST Webbook
log10ws	-3.42		Crippen Method
logp	3.613		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2660.00	kPa	KDB
rinpol	1025.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	1027.10		NIST Webbook
rinpol	978.10		NIST Webbook
rinpol	982.20		NIST Webbook
rinpol	985.20		NIST Webbook

rinpol	983.10		NIST Webbook
rinpol	1014.10		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1014.10		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	988.00		NIST Webbook
ripol	1088.00		NIST Webbook
ripol	1062.00		NIST Webbook
ripol	1075.00		NIST Webbook
tb	444.70	K	NIST Webbook
tb	444.90 ± 0.50	K	NIST Webbook
tb	444.70	K	NIST Webbook
tb	444.74 ± 0.03	K	NIST Webbook
tb	440.20	K	NIST Webbook
tb	444.69 ± 0.20	K	NIST Webbook
tb	444.70	K	KDB
tc	659.00	K	NIST Webbook
tc	659.00	K	KDB
tc	652.00	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	232.00	K	KDB
tf	231.95 ± 0.20	K	NIST Webbook
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.64	J/mol×K	619.69	Joback Method
cpg	301.81	J/mol×K	444.52	Joback Method
cpg	323.14	J/mol×K	479.55	Joback Method
cpg	343.23	J/mol×K	514.59	Joback Method
cpg	362.15	J/mol×K	549.62	Joback Method
cpg	379.94	J/mol×K	584.66	Joback Method
cpg	412.31	J/mol×K	654.72	Joback Method
cpl	264.80	J/mol×K	313.00	NIST Webbook
dvisc	0.0002719	Pa×s	444.52	Joback Method
dvisc	0.0145506	Pa×s	212.26	Joback Method
dvisc	0.0044939	Pa×s	250.97	Joback Method
dvisc	0.0019000	Pa×s	289.68	Joback Method

dvisc	0.0009840	Pa×s	328.39	Joback Method
dvisc	0.0005855	Pa×s	367.10	Joback Method
dvisc	0.0003846	Pa×s	405.81	Joback Method
hvapt	42.40 ± 0.10	kJ/mol	368.00	NIST Webbook
hvapt	37.01	kJ/mol	444.70	NIST Webbook
hvapt	42.90	kJ/mol	400.50	NIST Webbook
hvapt	45.00 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	44.00 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	43.00 ± 0.10	kJ/mol	358.00	NIST Webbook
rhol	813.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32339e+01
Coeff. B	-3.15642e+03
Coeff. C	-7.76360e+01
Temperature range (K), min.	321.45
Temperature range (K), max.	476.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.63471e+01
Coeff. B	-8.58272e+03
Coeff. C	-1.03859e+01
Coeff. D	4.50963e-06
Temperature range (K), min.	273.15
Temperature range (K), max.	659.00

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

Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
Solubility of 9-fluorenone, thianthrene and xanthene in organic solvents:	https://www.doi.org/10.1016/j.fluid.2005.02.016
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3178221&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=587
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol587.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume