Cyclohexane, propyl-

Other names:	1-cyclohexylpropane
	Cyclohexane, n-propyl-
	PROPYLCYCLOHEXANE
	n-Propylcyclohexane
Inchi:	InChI=1S/C9H18/c1-2-6-9-7-4-3-5-8-9/h9H,2-8H2,1H3
InchiKey:	DEDZSLCZHWTGOR-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CCCC1CCCCC1
Mol. weight [g/mol]:	126.24
CAS:	1678-92-8

Physical Properties

Property code	Value	Unit	Source
af	0.2580		KDB
ap	322.950	K	KDB
chl	-5875.80 ± 1.10	kJ/mol	NIST Webbook
chl	-5876.60 ± 0.92	kJ/mol	NIST Webbook
gf	47.35	kJ/mol	KDB
hcg	5875.76	kJ/mol	KDB
hcn	5479.660	kJ/mol	KDB
hf	-193.40	kJ/mol	KDB
hf	-193.30 ± 1.30	kJ/mol	NIST Webbook
hf	-192.40	kJ/mol	NIST Webbook
hfl	-237.50 ± 1.10	kJ/mol	NIST Webbook
hfl	-238.40 ± 1.30	kJ/mol	NIST Webbook
hfus	10.90	kJ/mol	Joback Method
hvap	44.70 ± 0.40	kJ/mol	NIST Webbook
hvap	45.10	kJ/mol	NIST Webbook
hvap	45.08	kJ/mol	NIST Webbook
hvap	45.10	kJ/mol	NIST Webbook
hvap	45.20	kJ/mol	NIST Webbook
hvap	42.80 ± 0.50	kJ/mol	NIST Webbook
hvap	44.70 ± 0.40	kJ/mol	NIST Webbook
hvap	45.10	kJ/mol	NIST Webbook
hvap	45.15	kJ/mol	NIST Webbook
hvap	45.20	kJ/mol	NIST Webbook
ie	9.46	eV	NIST Webbook

log10ws	-3.24		Crippen Method
logp	3.367		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2860.00	kPa	Critical Point Measurements for Five n-Alkylcyclohexanes (C6 to C10) by the Pulse-Heating Method
pc	2800.00	kPa	KDB
rinpol	931.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	930.50		NIST Webbook
rinpol	927.10		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	924.20		NIST Webbook

rinpol	927.10	NIST Webbook
rinpol	929.10	NIST Webbook
rinpol	936.40	NIST Webbook
rinpol	926.40	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	924.20	NIST Webbook
rinpol	927.10	NIST Webbook
rinpol	929.10	NIST Webbook
rinpol	927.10	NIST Webbook
rinpol	926.40	NIST Webbook
rinpol	925.22	NIST Webbook
rinpol	920.09	NIST Webbook
rinpol	923.67	NIST Webbook
rinpol	925.93	NIST Webbook
rinpol	925.46	NIST Webbook
rinpol	929.15	NIST Webbook
rinpol	931.59	NIST Webbook
rinpol	923.00	NIST Webbook
rinpol	933.00	NIST Webbook
rinpol	950.33	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	936.00	NIST Webbook
rinpol	935.00	NIST Webbook
rinpol	930.00	NIST Webbook
rinpol	944.00	NIST Webbook
rinpol	938.00	NIST Webbook
rinpol	939.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	936.40	NIST Webbook
rinpol	931.00	NIST Webbook
rinpol	937.00	NIST Webbook
rinpol	937.00	NIST Webbook
rinpol	933.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	923.00	NIST Webbook
rinpol	936.00	NIST Webbook
rinpol	962.10	NIST Webbook
rinpol	952.30	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	951.00	NIST Webbook
rinpol	938.00	NIST Webbook
rinpol	915.00	NIST Webbook
rinpol	926.40	NIST Webbook
rinpol	938.00	NIST Webbook

ripol	1003.00		NIST Webbook
ripol	1019.00		NIST Webbook
ripol	1019.00		NIST Webbook
ripol	1008.00		NIST Webbook
ripol	982.00		NIST Webbook
ripol	998.00		NIST Webbook
ripol	982.00		NIST Webbook
sg	419.86	J/mol×K	NIST Webbook
sl	311.88	J/mol×K	NIST Webbook
tb	429.90	K	KDB
tc	639.00	K	KDB
tc	630.80	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	178.06 ± 0.10	K	NIST Webbook
tf	178.19 ± 0.02	K	NIST Webbook
tf	178.09 ± 0.20	K	NIST Webbook
tf	178.70	K	KDB
tt	178.25 ± 0.02	K	NIST Webbook
vc	0.472	m3/kmol	KDB
zc	0.2490130		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.31	J/mol×K	524.34	Joback Method
cpg	339.46	J/mol×K	590.65	Joback Method
cpg	353.84	J/mol×K	623.81	Joback Method
cpg	291.49	J/mol×K	491.18	Joback Method
cpg	273.81	J/mol×K	458.03	Joback Method
cpg	255.25	J/mol×K	424.87	Joback Method
cpg	324.30	J/mol×K	557.50	Joback Method
cpl	242.04	J/mol×K	298.15	NIST Webbook
dvisc	0.0014438	Pa×s	274.00	Joback Method
dvisc	0.0008196	Pa×s	311.72	Joback Method
dvisc	0.0002741	Pa×s	424.87	Joback Method
dvisc	0.0005258	Pa×s	349.44	Joback Method
dvisc	0.0003678	Pa×s	387.15	Joback Method
dvisc	0.0030472	Pa×s	236.29	Joback Method
dvisc	0.0085410	Pa×s	198.57	Joback Method
hfust	10.60	kJ/mol	178.00	NIST Webbook

hfust	13.07	kJ/mol	178.25	NIST Webbook
hfust	10.37	kJ/mol	178.30	NIST Webbook
hfust	10.37	kJ/mol	178.30	NIST Webbook
hvapt	36.07	kJ/mol	429.90	KDB
hvapt	41.70	kJ/mol	388.50	NIST Webbook
rfi	1.43478		298.15	KDB
rhol	762.09	kg/m3	333.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	777.88	kg/m3	313.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	785.72	kg/m3	303.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	789.63	kg/m3	298.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	793.53	kg/m3	293.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhol	797.42	kg/m3	288.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	738.00	kg/m3	363.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	746.10	kg/m3	353.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	754.20	kg/m3	343.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane

rhol	762.12	kg/m3	333.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane	
rhol	770.00	kg/m3	323.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations	
rhol	770.04	kg/m3	323.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane	
rhol	777.90	kg/m3	313.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane	

rhol	785.73	kg/m3	303.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	793.54	kg/m3	293.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	793.00	kg/m3	293.00	KDB
sfust	58.19	J/mol×K	178.25	NIST Webbook
srf	0.03	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40078e+01
Coeff. B	-3.53909e+03
Coeff. C	-5.20770e+01
Temperature range (K), min.	310.03
Temperature range (K), max.	459.04

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	7.62408e+01
Coeff. B	-7.87048e+03
Coeff. C	-8.90935e+00
Coeff. D	3.80979e-06
Temperature range (K), min.	178.28
Temperature range (K), max.	639.15

Datasets

Thermal conductivity, W/m/K

Pressure, kPa - Gas	Temperature, K - Gas	Thermal conductivity, W/m/K - Gas
83.00	481.25	0.0276
83.00	481.94	0.0281
83.00	482.22	0.0282
84.00	481.45	0.0279
84.00	481.68	0.0280
88.00	453.61	0.0248
89.00	453.38	0.0247
89.00	453.87	0.0249
89.00	454.16	0.0250
90.00	454.48	0.0251
91.00	543.05	0.0361
91.00	543.18	0.0364
91.00	543.33	0.0367
91.00	543.51	0.0367
91.00	543.71	0.0367
120.00	510.63	0.0315
121.00	510.81	0.0317
121.00	511.02	0.0319
121.00	511.26	0.0319
124.00	603.12	0.0448
124.00	603.25	0.0448
125.00	603.40	0.0450
125.00	603.55	0.0448
125.00	603.73	0.0447
131.00	481.93	0.0283
131.00	482.21	0.0283

131.00	573.95	0.0403
132.00	481.23	0.0280
132.00	481.43	0.0282
132.00	481.66	0.0283
132.00	573.62	0.0403
132.00	573.78	0.0403
150.00	453.32	0.0246
150.00	453.55	0.0248
151.00	453.82	0.0249
151.00	603.10	0.0461
151.00	603.16	0.0462
151.00	603.22	0.0461
151.00	603.29	0.0461
151.00	603.36	0.0459
152.00	603.43	0.0459
152.00	603.49	0.0458
153.00	454.11	0.0250
153.00	603.56	0.0461
154.00	454.43	0.0251
154.00	603.63	0.0462
154.00	603.71	0.0463
162.00	453.23	0.0249
163.00	453.47	0.0250
163.00	453.73	0.0251
164.00	454.03	0.0251
164.00	454.35	0.0252
191.00	481.24	0.0289
192.00	481.44	0.0289
193.00	481.65	0.0290
193.00	481.89	0.0290
193.00	482.17	0.0290
213.00	511.24	0.0323
214.00	510.62	0.0318
214.00	510.81	0.0319
214.00	511.02	0.0321
222.00	543.02	0.0365
224.00	543.16	0.0370
226.00	543.32	0.0371
227.00	543.49	0.0371
228.00	543.70	0.0369
248.00	481.29	0.0288
248.00	481.48	0.0288
249.00	481.69	0.0290
250.00	481.92	0.0290

251.00	482.18	0.0291
259.00	573.47	0.0405
260.00	573.61	0.0406
261.00	573.77	0.0408
262.00	573.95	0.0408
287.00	603.17	0.0467
289.00	603.28	0.0470
290.00	603.41	0.0473
291.00	603.57	0.0472
310.00	481.26	0.0290
310.00	481.45	0.0292
310.00	481.65	0.0293
310.00	481.88	0.0295
310.00	482.13	0.0296
312.00	510.40	0.0330
312.00	510.56	0.0331
312.00	510.74	0.0332
312.00	510.96	0.0332
312.00	511.19	0.0331
320.00	543.01	0.0372
321.00	543.15	0.0376
322.00	543.31	0.0376
322.00	543.49	0.0374
322.00	543.70	0.0372
411.00	573.71	0.0420
412.00	510.73	0.0337
412.00	573.43	0.0417
412.00	573.56	0.0420
413.00	510.38	0.0340
413.00	510.55	0.0339
413.00	510.93	0.0338
413.00	511.14	0.0338
413.00	573.30	0.0416
413.00	573.86	0.0420
428.00	542.99	0.0380
428.00	543.65	0.0380
429.00	543.13	0.0383
429.00	543.28	0.0385
429.00	543.46	0.0380
502.00	603.20	0.0457
503.00	603.33	0.0460
504.00	603.46	0.0464
504.00	603.61	0.0466
508.00	510.36	0.0349

508.00	510.51	0.0348
509.00	510.68	0.0348
510.00	510.86	0.0347
511.00	511.07	0.0347
514.00	542.99	0.0387
515.00	543.11	0.0389
516.00	543.24	0.0391
517.00	543.39	0.0390
518.00	543.56	0.0391
562.00	573.29	0.0427
562.00	573.41	0.0426
563.00	573.52	0.0429
565.00	573.64	0.0433
567.00	573.77	0.0437
656.00	542.99	0.0380
656.00	543.13	0.0380
657.00	543.27	0.0382
658.00	543.42	0.0385
659.00	543.58	0.0388

Reference *https://www.doi.org/10.1021/je800255r*

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Critical Point Measurements for Five n-Alkylcyclohexanes (C6 to C10) by the Pulse Heating Method:	https://www.doi.org/10.1021/je0256535
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1678928&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol559.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=559
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Heptyl-, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane from 300 K to 600 K at Pressures to 60 MPa:	https://www.doi.org/10.1021/acs.jced.8b00692
Measurement and correlation of the thermal conductivity of n-Hexadecane and n-Dodecane at pressures up to 60 MPa:	https://www.doi.org/10.1021/je800255r
KDB Pure (Korean Thermophysical Properties Database):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=559
Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations:	https://www.doi.org/10.1021/acs.jced.8b01135
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
hfl:	Liquid phase 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
tcondg:	Gas thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility