Cyclohexane, hexyl-

Other names:	1-CYCLOHEXYLHEXANE
	1-HEXYLCYCLOHEXANE
	Cyclohexane, n-hexyl-
	HEXYLCYCLOHEXANE
	Hexane, 1-cyclohexyl-
	n-Hexylcyclohexane
Inchi:	InChI=1S/C12H24/c1-2-3-4-6-9-12-10-7-5-8-11-12/h12H,2-11H2,1H3
InchiKey:	QHWAQXOSHHKCFK-UHFFFAOYSA-N
Formula:	C12H24
SMILES:	CCCCCCC1CCCCC1
Mol. weight [g/mol]:	168.32
CAS:	4292-75-5

Physical Properties

Property code	Value	Unit	Source
af	0.4560		KDB
chl	-7897.80 ± 1.60	kJ/mol	NIST Webbook
gf	74.61	kJ/mol	Joback Method
hf	-254.40 ± 1.80	kJ/mol	NIST Webbook
hfus	18.67	kJ/mol	Joback Method
hvap	58.95 ± 0.50	kJ/mol	NIST Webbook
hvap	59.00 ± 0.50	kJ/mol	NIST Webbook
hvap	55.90 ± 0.50	kJ/mol	NIST Webbook
hvap	59.90	kJ/mol	NIST Webbook
log10ws	-4.50		Crippen Method
logp	4.537		Crippen Method
mcvol	169.080	ml/mol	McGowan Method
pc	2130.00	kPa	KDB
rinpol	1243.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1233.00		NIST Webbook

rinpol	1259.00		NIST Webbook
rinpol	1233.90		NIST Webbook
rinpol	1237.70		NIST Webbook
rinpol	1239.50		NIST Webbook
rinpol	1237.70		NIST Webbook
rinpol	1237.10		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1233.90		NIST Webbook
rinpol	1237.70		NIST Webbook
rinpol	1239.50		NIST Webbook
rinpol	1237.70		NIST Webbook
rinpol	1237.10		NIST Webbook
rinpol	1231.08		NIST Webbook
rinpol	1235.37		NIST Webbook
rinpol	1238.08		NIST Webbook
rinpol	1237.21		NIST Webbook
rinpol	1241.62		NIST Webbook
rinpol	1244.73		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1246.00		NIST Webbook
ripol	1309.40		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1293.20		NIST Webbook
ripol	1287.60		NIST Webbook
ripol	1320.40		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1315.10		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1298.60		NIST Webbook
ripol	1304.10		NIST Webbook
ripol	1322.00		NIST Webbook
tb	497.93 ± 0.50	K	NIST Webbook
tb	494.15 ± 2.00	K	NIST Webbook
tb	497.90	K	KDB
tb	493.15 ± 2.00	K	NIST Webbook
tb	497.93 ± 0.20	K	NIST Webbook
tb	497.80 ± 0.60	K	NIST Webbook
tc	691.80	K	KDB
tf	225.64 ± 0.20	K	NIST Webbook
tf	225.64 ± 0.50	K	NIST Webbook
tf	264.00	K	KDB
vc	0.640	m3/kmol	KDB

zc	0.2371820	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.17	J/mol×K	493.51	Joback Method
cpg	416.07	J/mol×K	525.55	Joback Method
cpg	435.98	J/mol×K	557.59	Joback Method
cpg	454.91	J/mol×K	589.64	Joback Method
cpg	472.89	J/mol×K	621.68	Joback Method
cpg	489.96	J/mol×K	653.72	Joback Method
cpg	506.14	J/mol×K	685.76	Joback Method
dvisc	0.0082624	Pa×s	232.38	Joback Method
dvisc	0.0028566	Pa×s	275.90	Joback Method
dvisc	0.0013191	Pa×s	319.42	Joback Method
dvisc	0.0007331	Pa×s	362.94	Joback Method
dvisc	0.0004621	Pa×s	406.47	Joback Method
dvisc	0.0003184	Pa×s	449.99	Joback Method
dvisc	0.0002343	Pa×s	493.51	Joback Method
hvapt	42.84	kJ/mol	497.90	KDB
rhol	807.71	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	800.56	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	793.40	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	786.22	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	779.02	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	771.80	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	764.60	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	757.30	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	811.34	kg/m3	288.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhol	807.76	kg/m3	293.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	804.19	kg/m3	298.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	800.61	kg/m3	303.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	793.43	kg/m3	313.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	786.25	kg/m3	323.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhol	779.05	kg/m3	333.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42234e+01
Coeff. B	-4.00982e+03
Coeff. C	-8.03920e+01
Temperature range (K), min.	368.13
Temperature range (K), max.	530.33

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.05859e+02
Coeff. B	-1.07629e+04
Coeff. C	-1.30421e+01
Coeff. D	5.52864e-06
Temperature range (K), min.	265.15
Temperature range (K), max.	691.81

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol592.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4292755&Units=SI
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:	https://www.doi.org/10.1021/acs.jced.8b00692
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=592

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
zc:	Critical Compressibility