Cyclohexane, decyl-

Other names:	1-CYCLOHEXYLDECANE 1-DECYLCYCLOHEXANE Cyclohexane, n-decyl- DECYLCYCLOHEXANE Decane, 1-cyclohexyl- n-Decylcyclohexane
Inchi:	InChI=1S/C16H32/c1-2-3-4-5-6-7-8-10-13-16-14-11-9-12-15-16/h16H,2-15H2,1H3
InchiKey:	STWFZICHPLEOIC-UHFFFAOYSA-N
Formula:	C16H32
SMILES:	CCCCCCCCCCC1CCCCC1
Mol. weight [g/mol]:	224.43
CAS:	1795-16-0

Physical Properties

Property code	Value	Unit	Source
af	0.6130		KDB
chl	-10451.10 ± 3.30	kJ/mol	NIST Webbook
chl	-10451.20 ± 1.80	kJ/mol	NIST Webbook
chl	-10532.80 ± 2.20	kJ/mol	NIST Webbook
gf	108.29	kJ/mol	Joback Method
hf	-336.90 ± 2.40	kJ/mol	NIST Webbook
hfl	-418.40 ± 2.10	kJ/mol	NIST Webbook
hfus	29.03	kJ/mol	Joback Method
hvap	78.76	kJ/mol	NIST Webbook
hvap	79.70	kJ/mol	NIST Webbook
hvap	78.70 ± 0.80	kJ/mol	NIST Webbook
log10ws	-6.17		Crippen Method
logp	6.098		Crippen Method
mcvol	225.440	ml/mol	McGowan Method
pc	1540.00	kPa	KDB
rinpol	1656.20		NIST Webbook
rinpol	1656.20		NIST Webbook
rinpol	1655.90		NIST Webbook
rinpol	1650.70		NIST Webbook
rinpol	1656.20		NIST Webbook
rinpol	1658.40		NIST Webbook
rinpol	1650.70		NIST Webbook

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rinpol	1656.00		NIST Webbook
rinpol	1655.90		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1653.53		NIST Webbook
rinpol	1656.86		NIST Webbook
rinpol	1655.41		NIST Webbook
rinpol	1660.95		NIST Webbook
rinpol	1664.11		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1648.54		NIST Webbook
sg	694.42	J/mol×K	NIST Webbook
tb	560.00 ± 3.00	K	NIST Webbook
tb	570.80	K	KDB
tc	750.00	K	KDB
tf	271.40 ± 0.04	K	NIST Webbook
tf	271.40 ± 0.04	K	NIST Webbook
tf	271.43 ± 0.03	K	NIST Webbook
tf	271.14 ± 0.40	K	NIST Webbook
tf	271.45 ± 0.50	K	NIST Webbook
tf	271.00	K	KDB
tt	271.43 ± 0.02	K	NIST Webbook
tt	271.42 ± 0.05	K	NIST Webbook
tt	271.44 ± 0.02	K	NIST Webbook
vc	0.865	m3/kmol	KDB
zc	0.2134950		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.97	J/mol×K	585.03	Joback Method
cpg	649.97	J/mol×K	646.25	Joback Method
cpg	670.38	J/mol×K	676.87	Joback Method
cpg	689.76	J/mol×K	707.48	Joback Method
cpg	708.16	J/mol×K	738.09	Joback Method
cpg	725.60	J/mol×K	768.70	Joback Method

cpg	628.52	J/mol×K	615.64	Joback Method
dvisc	0.0003308	Pa×s	482.51	Joback Method
dvisc	0.0005336	Pa×s	431.25	Joback Method
dvisc	0.0002248	Pa×s	533.77	Joback Method
dvisc	0.0021724	Pa×s	328.72	Joback Method
dvisc	0.0064682	Pa×s	277.46	Joback Method
dvisc	0.0001634	Pa×s	585.03	Joback Method
dvisc	0.0009794	Pa×s	379.98	Joback Method
hfust	38.62	kJ/mol	271.40	NIST Webbook
hfust	38.62	kJ/mol	271.40	NIST Webbook
hvapt	50.38	kJ/mol	570.80	KDB
hvapt	76.70	kJ/mol	398.00	NIST Webbook
hvapt	61.60	kJ/mol	520.00	NIST Webbook
rhol	819.00	kg/m3	293.00	KDB
rhol	798.26	kg/m3	323.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	805.02	kg/m3	313.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	791.49	kg/m3	333.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	811.78	kg/m3	303.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhol	815.16	kg/m3	298.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	818.54	kg/m3	293.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	821.93	kg/m3	288.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	764.40	kg/m3	373.15	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	771.20	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	778.00	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	784.80	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	791.50	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	798.27	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	805.02	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	811.78	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	818.55	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
srf	0.03	N/m	298.20	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	271.30	K	100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes

tfp	276.00	K	20000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	280.50	K	40100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	284.80	K	59900.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	289.20	K	80100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	293.90	K	100100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56565e+01
Coeff. B	-5.17811e+03
Coeff. C	-9.08880e+01
Temperature range (K), min.	427.81
Temperature range (K), max.	591.43

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.83202e+02
Coeff. B	-1.66574e+04
Coeff. C	-2.40646e+01
Coeff. D	1.02076e-05
Temperature range (K), min.	271.42
Temperature range (K), max.	751.25

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes:	https://www.doi.org/10.1021/je600575r
KDB:	https://www.cheric.org/files/research/kdb/mol/mol597.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=597
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795160&Units=SI
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

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
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
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
sg:	Molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility