Cyclohexane, octyl-

Other names:	1-Cyclohexyloctane
	Cyclohexane, n-octyl-
	Octane, 1-cyclohexyl-
	Octylcyclohexane
	n-Octylcyclohexane
	octane, 1-cyclohexyl
Inchi:	InChI=1S/C14H28/c1-2-3-4-5-6-8-11-14-12-9-7-10-13-14/h14H,2-13H2,1H3
InchiKey:	FBXWCEKQCVOOLT-UHFFFAOYSA-N
Formula:	C14H28
SMILES:	CCCCCCCCC1CCCCC1
Mol. weight [g/mol]:	196.37
CAS:	1795-15-9

Physical Properties

Property code	Value	Unit	Source
chl	-9215.30 ± 1.90	kJ/mol	NIST Webbook
gf	91.45	kJ/mol	Joback Method
hf	-295.60 ± 2.10	kJ/mol	NIST Webbook
hfus	23.85	kJ/mol	Joback Method
hvap	69.80	kJ/mol	NIST Webbook
log10ws	-5.34		Crippen Method
logp	5.317		Crippen Method
mcvol	197.260	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	1442.40		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1447.50		NIST Webbook
rinpol	1447.10		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1447.50		NIST Webbook
rinpol	1449.10		NIST Webbook

rinpol	1432.00		NIST Webbook
rinpol	1442.40		NIST Webbook
rinpol	1447.50		NIST Webbook
rinpol	1449.10		NIST Webbook
rinpol	1447.50		NIST Webbook
rinpol	1447.10		NIST Webbook
rinpol	1439.90		NIST Webbook
rinpol	1444.49		NIST Webbook
rinpol	1447.56		NIST Webbook
rinpol	1446.58		NIST Webbook
rinpol	1451.58		NIST Webbook
rinpol	1454.77		NIST Webbook
rinpol	1437.00		NIST Webbook
tb	528.00 ± 3.00	K	NIST Webbook
tc	726.99	K	Joback Method
tf	252.75 ± 0.50	K	NIST Webbook
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.65	J/mol×K	726.99	Joback Method
cpg	519.34	J/mol×K	570.56	Joback Method
cpg	540.18	J/mol×K	601.84	Joback Method
cpg	560.00	J/mol×K	633.13	Joback Method
cpg	578.83	J/mol×K	664.42	Joback Method
cpg	596.70	J/mol×K	695.70	Joback Method
cpg	497.45	J/mol×K	539.27	Joback Method
dvisc	0.0002721	Pa×s	491.88	Joback Method
dvisc	0.0003979	Pa×s	444.49	Joback Method
dvisc	0.0006371	Pa×s	397.10	Joback Method
dvisc	0.0011589	Pa×s	349.70	Joback Method
dvisc	0.0025428	Pa×s	302.31	Joback Method
dvisc	0.0001990	Pa×s	539.27	Joback Method
dvisc	0.0074728	Pa×s	254.92	Joback Method
hvapt	62.70	kJ/mol	383.00	NIST Webbook

rhol	772.50	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	779.50	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	817.58	kg/m3	288.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	814.13	kg/m3	293.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	810.67	kg/m3	298.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhol	807.21	kg/m3	303.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	800.28	kg/m3	313.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	793.35	kg/m3	323.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	786.41	kg/m3	333.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	807.20	kg/m3	303.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhol	786.42	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	793.36	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	800.29	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	807.22	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	814.14	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	765.50	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	758.50	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52442e+01
Coeff. B	-4.79325e+03

Coeff. C	-7.69060e+01
Temperature range (K), min.	397.38
Temperature range (K), max.	559.48

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795159&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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