Cyclooctane

Other names:	292-64-8
	OCTAMETHYLENE
Inchi:	InChI=1S/C8H16/c1-2-4-6-8-7-5-3-1/h1-8H2
InchiKey:	WJTCGQSWYFHTAC-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	C1CCCCCCC1
Mol. weight [g/mol]:	112.21
CAS:	292-64-8

Physical Properties

Property code	Value	Unit	Source
af	0.2360		KDB
chl	-5265.30 ± 1.60	kJ/mol	NIST Webbook
chl	-5265.70 ± 0.90	kJ/mol	NIST Webbook
chs	-5252.60	kJ/mol	NIST Webbook
gf	24.44	kJ/mol	Joback Method
hcg	5265.56	kJ/mol	KDB
hcn	4913.690	kJ/mol	KDB
hf	-126.10 ± 1.60	kJ/mol	NIST Webbook
hfl	-169.40 ± 1.60	kJ/mol	NIST Webbook
hfus	3.04	kJ/mol	Joback Method
hvap	43.35 ± 0.21	kJ/mol	NIST Webbook
hvap	44.70	kJ/mol	NIST Webbook
hvap	43.30 ± 0.20	kJ/mol	NIST Webbook
hvap	43.50	kJ/mol	NIST Webbook
ie	9.75	eV	NIST Webbook
ie	9.82 ± 0.05	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	10.08 ± 0.05	eV	NIST Webbook
ie	9.74 ± 0.05	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.75 ± 0.04	eV	NIST Webbook
log10ws	-4.15		Estimated Solubility Method
log10ws	-4.15		Aqueous Solubility Prediction Method
logp	3.121		Crippen Method
mcvol	112.720	ml/mol	McGowan Method

pc	3560.00 ± 40.00	kPa	NIST Webbook
pc	3560.00 ± 40.53	kPa	NIST Webbook
pc	3550.00 ± 40.00	kPa	NIST Webbook
pc	3560.00	kPa	KDB
rhoc	273.80 ± 4.49	kg/m3	NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	965.80		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	963.90		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	927.20		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	928.50		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	925.00		NIST Webbook

rinpol	927.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	930.00		NIST Webbook
ripol	1036.00		NIST Webbook
ripol	1014.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1023.00		NIST Webbook
ripol	1036.00		NIST Webbook
sg	366.80 ± 1.30	J/mol×K	NIST Webbook
sl	262.00	J/mol×K	NIST Webbook
tb	423.85 ± 0.30	K	NIST Webbook
tb	416.00 ± 4.00	K	NIST Webbook
tb	425.15 ± 2.00	K	NIST Webbook
tb	416.15 ± 5.00	K	NIST Webbook
tb	423.15 ± 1.00	K	NIST Webbook
tb	420.80 ± 1.00	K	NIST Webbook
tb	422.70 ± 1.00	K	NIST Webbook
tb	424.12 ± 0.30	K	NIST Webbook
tb	423.30 ± 0.50	K	NIST Webbook
tb	422.00	K	KDB
tc	647.20 ± 0.50	K	NIST Webbook
tc	674.20 ± 0.60	K	NIST Webbook
tc	647.20 ± 0.50	K	NIST Webbook
tc	647.50	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	647.20	K	KDB
tf	287.74 ± 0.10	K	NIST Webbook
tf	281.75 ± 4.00	K	NIST Webbook
tf	286.90 ± 1.50	K	NIST Webbook
tf	282.90 ± 3.00	K	NIST Webbook
tf	287.98	K	KDB
tf	281.90 ± 3.00	K	NIST Webbook
tf	284.20 ± 5.00	K	NIST Webbook
tf	287.50 ± 0.60	K	NIST Webbook
tf	287.65 ± 0.30	K	NIST Webbook
tf	287.08	K	Aqueous Solubility Prediction Method
tf	284.90 ± 2.00	K	NIST Webbook
tf	287.82 ± 0.10	K	NIST Webbook
tt	287.94 ± 0.07	K	NIST Webbook
tt	287.98 ± 0.05	K	NIST Webbook
tt	287.94 ± 0.05	K	NIST Webbook

tt	288.00 ± 3.00	K	NIST Webbook
tt	287.97 ± 0.02	K	NIST Webbook
vc	0.410	m3/kmol	NIST Webbook
vc	0.411 ± 0.007	m3/kmol	NIST Webbook
vc	0.410	m3/kmol	KDB
zc	0.2712430		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.35	J/mol×K	597.61	Joback Method
cpg	230.16	J/mol×K	451.68	Joback Method
cpg	266.16	J/mol×K	524.64	Joback Method
cpg	248.64	J/mol×K	488.16	Joback Method
cpg	282.72	J/mol×K	561.12	Joback Method
cpg	313.06	J/mol×K	634.09	Joback Method
cpg	210.69	J/mol×K	415.20	Joback Method
cpl	215.53	J/mol×K	298.15	NIST Webbook
cpl	215.78	J/mol×K	298.15	NIST Webbook
cpl	214.53	J/mol×K	298.15	NIST Webbook
cpl	214.24	J/mol×K	298.15	NIST Webbook
cpl	215.48	J/mol×K	298.15	NIST Webbook
cpl	215.46	J/mol×K	298.15	NIST Webbook
dvisc	0.0016360	Pa×s	313.15	Viscometric and Volumetric Properties of 10 Regular Binary Systems at 308.15 K and 313.15 K
dvisc	0.0018026	Pa×s	308.15	Viscometric and Volumetric Properties of 10 Regular Binary Systems at 308.15 K and 313.15 K
hfust	0.48	kJ/mol	183.80	NIST Webbook
hfust	6.32	kJ/mol	166.50	NIST Webbook
hfust	2.41	kJ/mol	288.00	NIST Webbook
hfust	2.41	kJ/mol	288.00	NIST Webbook
hsubt	58.70	kJ/mol	166.00	NIST Webbook
hvapt	40.30	kJ/mol	385.50	NIST Webbook
hvapt	43.10	kJ/mol	307.00	NIST Webbook
hvapt	39.30	kJ/mol	403.50	NIST Webbook

hvapt	43.30	kJ/mol	329.00	NIST Webbook
hvapt	39.40	kJ/mol	418.00	NIST Webbook
rfi	1.45598		298.15	Separation of toluene from cyclic hydrocarbons using 1-butyl-3-methylimidazolium methylsulfate ionic liquid at T = 298.15 K and atmospheric pressure
rfi	1.45598		298.15	Liquid Extraction of Benzene from Its Mixtures Using 1-Ethyl-3-methylimidazolium Ethylsulfate as a Solvent
rfi	1.45598		298.15	Extraction of Benzene from Aliphatic Compounds Using Commercial Ionic Liquids as Solvents: Study of the Liquid Liquid Equilibrium at T = 298.15 K
rfi	1.45598		298.15	(Liquid + liquid) equilibrium data for the ternary systems (cycloalkane + ethylbenzene + 1-ethyl-3-methylimidazolium ethylsulfate) at T = 298.15 K and atmospheric pressure
rfi	1.45598		298.15	Density, Speed of Sound, and Refractive Index of the Binary Systems Cyclohexane (1) or Methylcyclohexane (1) or Cyclo-octane (1) with Benzene (2), Toluene (2), and Ethylbenzene (2) at Two Temperatures

rfi	1.45598		298.15	Density, Speed of Sound, and Refractive Index for Binary Mixtures Containing Cycloalkanes with o-Xylene, m-Xylene, p-Xylene, and Mesitylene at T = (298.15 and 313.15) K
rfi	1.44877		313.15	Density, Speed of Sound, and Refractive Index for Binary Mixtures Containing Cycloalkanes with o-Xylene, m-Xylene, p-Xylene, and Mesitylene at T = (298.15 and 313.15) K
rfi	1.45598		298.15	Experimental data, correlation and prediction of the extraction of benzene from cyclic hydrocarbons using [Epy][ESO4] ionic liquid
rfi	1.45624		298.15	Liquid liquid equilibria of lactam containing binary systems
rfi	1.45598		298.15	Liquid Liquid Extraction of Aromatic Compounds from Cycloalkanes Using 1-Butyl-3-methylimidazolium Methylsulfate Ionic Liquid
rfi	1.45630		298.15	KDB
rhol	831.87	kg/m3	298.15	Thermodynamics of Mixtures Containing a Very Strongly Polar Compound. 10. Liquid Liquid Equilibria for N,N-Dimethylacetamide + Selected Alkanes

rhol	831.47	kg/m3	298.15	Evaluation of ionic liquids as solvent for aromatic extraction: Experimental, correlation and COSMO-RS predictions
rhol	834.00	kg/m3	293.00	KDB
sfust	8.35	J/mol×K	288.00	NIST Webbook
sfust	37.94	J/mol×K	166.50	NIST Webbook
sfust	2.60	J/mol×K	183.80	NIST Webbook
srf	0.03	N/m	293.20	KDB
tcondl	0.12	W/m×K	296.09	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	295.88	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	295.85	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	296.21	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	289.17	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	288.96	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	288.70	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	311.67	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	311.88	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.12	W/m×K	312.10	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	328.99	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	329.22	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	329.43	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.20	K	98.70	NIST Webbook
tbrp	421.70	K	99.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45798e+01
Coeff. B	-3.61720e+03
Coeff. C	-5.52360e+01
Temperature range (K), min.	303.15
Temperature range (K), max.	445.51

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.82856e+01
Coeff. B	-7.74858e+03
Coeff. C	-9.30682e+00
Coeff. D	5.02648e-06
Temperature range (K), min.	367.00
Temperature range (K), max.	647.20

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	298.15	831.61

Reference *https://www.doi.org/10.1016/j.jct.2017.09.027*

Sources

Measurement of activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium 2-(2-methoxyethoxy) ethylsulfate at T = (308.15, 313.15, 323.15 and 333.15) K using gas + liquid chromatography: https://www.doi.org/10.1016/j.jct.2013.10.017

Thermodynamics and activity coefficients at infinite dilution for organic solutes, water and diols in the ionic liquid choline bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2014.04.024
The Critical Temperatures of a Number of (i) (Chloroalkane (C3 C4) + Hydrocarbon (C6 C8)) Binary Mixtures and (ii) (Aromatic Halocarbon (Chlorobenzene, Fluorobenzene, 1,2-Dichlorobenzene, or 1,3-Dichlorobenzene) + Alkane (C8)) Binary Mixtures	https://www.doi.org/10.1021/acs.jced.7b00191
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Activity Coefficients at Infinite Dilution of Organic Solutes and Water in Tributylethylphosphonium Diethylphosphate Using Gas Liquid Chromatography: Thermodynamic Properties of Mixtures Containing Ionic Liquids:	https://www.doi.org/10.1021/acs.jced.5b00980
Activity Coefficients at Infinite Dilution of Various Solutes in [illegible] Deep Eutectic Solvent [illegible]	https://www.doi.org/10.1021/acs.jced.8b00600
Activity Coefficients at Infinite Dilution Measurements for Organic Solutes and Water in the Ionic Liquid 1-Butyl-3-methyl-pyridinium Trifluoromethanesulfonate:	https://www.doi.org/10.1021/je1000582
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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Density, Speed of Sound, and Refractive Index of the Binary Systems Cyclohexane (1) or Methylcyclohexane (1) or Cyclo-octane (1) with Benzene (2), Toluene (2), and Ethylbenzene (2) at Two Temperatures:	https://www.doi.org/10.1021/je900468u
Infinite dilution activity coefficients, specific retention volumes and [illegible] hydrocarbons in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
High selective water/butan-1-ol separation on investigation of limiting activity coefficients with [P8,8,8,8][NTf2] ionic liquid:	https://www.doi.org/10.1016/j.fluid.2017.06.001
Ammonium-based ionic liquids in extraction of butan-1-ol from water phase using activity coefficients at infinite dilution:	https://www.doi.org/10.1016/j.fluid.2018.09.024
Separation of aliphatic from aromatic hydrocarbons and sulphur compounds from fuel based on measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid N,N-diethyl-N-methyl-N-(2-methoxy-ethyl)ammonium bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2016.07.017
Determination of Activity Coefficients at Infinite Dilution of 35 Solutes in the Ionic Liquid 1-Butyl-3-methylimidazolium Tosylate, using Gas-Liquid Chromatography	https://www.doi.org/10.1021/je100410k
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-butyl-3-methylimidazolium hexafluoroantimonate using gas-liquid chromatography at T = (313.15, 323.15, and 333.15) K:	https://www.doi.org/10.1016/j.jct.2010.12.019
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium trifluoromethanesulfonate using gas liquid chromatography at T = (313.15, 323.15, and 333.15) K:	https://www.doi.org/10.1016/j.jct.2009.07.010
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Application of [EMIm][ESO4] ionic liquid as solvent in the extraction of toluene from cycloalkanes: Study of liquid-liquid equilibria at T = 298.15 K:	https://www.doi.org/10.1016/j.fluid.2011.01.021
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The study of activity coefficients at infinite dilution for organic solutes and water in 1-butyl-[illegible] [illegible][FAP] [illegible]	https://www.doi.org/10.1016/j.jct.2013.09.007
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Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
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Liquid Extraction of Benzene from Its Mixtures Using [illegible]	https://www.doi.org/10.1021/je100508y
Tetramethylammonium chloride + glycerol deep eutectic solvent as separation agent for organic liquid mixtures: Assessment from experimental limiting activity coefficients:	https://www.doi.org/10.1016/j.fluid.2018.06.003
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Thermodynamics of mixtures containing aromatic nitriles:	https://www.doi.org/10.1016/j.jct.2017.09.027
A 1-alkylcyanopyridinium-based ionic liquid in the separation processes:	https://www.doi.org/10.1016/j.jct.2016.01.017
(Liquid + liquid) equilibrium data for the ternary systems (cycloalkane + ethylbenzene +	https://www.doi.org/10.1016/j.jct.2010.12.014
Activity coefficients at infinite dilution measurements for organic solutes in [EMIM][SCN] ionic liquid	https://www.doi.org/10.1016/j.fluid.2008.10.008
Ethylsulfate) at T = 298.15 K and	https://www.cheric.org/files/research/kdb/mol/mol503.mol
N-butyl-4-methylpyridinium tosylate ionic liquid: Effect of temperature and	https://www.doi.org/10.1016/j.fluid.2013.10.033
Using GLC at T = 328.15, 338.15, 348.15, and 343.15K	https://www.doi.org/10.1016/j.jct.2018.02.014
[EMIM][SO4] ionic liquid:	https://www.doi.org/10.1021/je0498107
Nonpolar Solutes in the Ionic Liquid	https://www.doi.org/10.1016/j.jct.2018.07.024
1-Ethyl-3-methylimidazolium ethylsulfate:	https://www.doi.org/10.1016/j.jct.2013.05.030
Using Gas−Liquid Chromatography at	https://www.doi.org/10.1021/je901020a
Gas−liquid chromatography at 313.15 K:	https://www.doi.org/10.1016/j.jct.2013.07.011
Measurements of Activity Coefficients at Infinite Dilution of Solutes	https://www.doi.org/10.1016/j.fluid.2009.12.019
Activity coefficients at Infinite Dilution Measurements for Organic Solutes and	https://www.doi.org/10.1021/je900890u
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Separation of binary mixtures	https://www.doi.org/10.1016/j.jct.2017.03.004

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid 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
hsubt:	Enthalpy of sublimation 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
rhoc:	Critical density
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility