

Cyclohexane, ethyl-

Other names:	Ethylcyclohexane
Inchi:	InChI=1S/C8H16/c1-2-8-6-4-3-5-7-8/h8H,2-7H2,1H3
InchiKey:	IIEWJVIFRVWJOD-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CCC1CCCCC1
Mol. weight [g/mol]:	112.21
CAS:	1678-91-7

Physical Properties

Property code	Value	Unit	Source
af	0.2430		KDB
ap	316.950	K	KDB
chl	-5222.60 ± 1.50	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	39.27	kJ/mol	KDB
hcg	5222.59	kJ/mol	KDB
hcn	4870.511	kJ/mol	KDB
hf	-172.60	kJ/mol	NIST Webbook
hf	-171.80 ± 1.50	kJ/mol	NIST Webbook
hf	-171.90	kJ/mol	KDB
hfl	-212.20 ± 1.50	kJ/mol	NIST Webbook
hfl	-213.00	kJ/mol	NIST Webbook
hfus	8.31	kJ/mol	Joback Method
hvap	33.83	kJ/mol	Joback Method
ie	9.67 ± 0.02	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
log10ws	-4.25		Estimated Solubility Method
log10ws	-4.25		Aqueous Solubility Prediction Method
logp	2.977		Crippen Method
mvol	112.720	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3000.00	kPa	KDB

pc

3250.00

kPa

Critical Point
Measurements for Five
n-Alkylcyclohexanes (C6
to C10) by the
Pulse-Heating Method

rinpol	867.90	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	837.00	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	846.00	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	829.00	NIST Webbook
rinpol	842.20	NIST Webbook
rinpol	859.70	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	828.00	NIST Webbook
rinpol	833.60	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	843.00	NIST Webbook
rinpol	834.30	NIST Webbook
rinpol	842.80	NIST Webbook
rinpol	831.30	NIST Webbook
rinpol	831.70	NIST Webbook
rinpol	853.00	NIST Webbook
rinpol	837.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	848.00	NIST Webbook
rinpol	842.00	NIST Webbook
rinpol	842.00	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	841.00	NIST Webbook
rinpol	844.00	NIST Webbook
rinpol	834.30	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	842.00	NIST Webbook
rinpol	825.00	NIST Webbook

rinpol	828.00	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	845.00	NIST Webbook
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rinpol	839.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	842.00	NIST Webbook
rinpol	835.92	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	843.00	NIST Webbook
rinpol	845.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	841.00	NIST Webbook
rinpol	832.20	NIST Webbook
rinpol	829.10	NIST Webbook
rinpol	828.40	NIST Webbook
rinpol	826.90	NIST Webbook
rinpol	829.10	NIST Webbook
rinpol	830.90	NIST Webbook
rinpol	838.10	NIST Webbook
rinpol	830.10	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	826.90	NIST Webbook
rinpol	829.10	NIST Webbook
rinpol	830.90	NIST Webbook
rinpol	829.10	NIST Webbook
rinpol	828.40	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	821.60	NIST Webbook
rinpol	824.96	NIST Webbook
rinpol	827.15	NIST Webbook
rinpol	827.11	NIST Webbook
rinpol	830.63	NIST Webbook
rinpol	832.99	NIST Webbook
rinpol	841.00	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	828.00	NIST Webbook
rinpol	833.00	NIST Webbook
rinpol	843.00	NIST Webbook
rinpol	833.00	NIST Webbook

rinpol	836.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	831.70		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	837.90		NIST Webbook
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rinpol	824.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	850.00		NIST Webbook
ripol	920.00		NIST Webbook
ripol	910.10		NIST Webbook
ripol	920.00		NIST Webbook
ripol	885.00		NIST Webbook
ripol	920.00		NIST Webbook
ripol	910.10		NIST Webbook
ripol	905.50		NIST Webbook
ripol	915.00		NIST Webbook
ripol	920.00		NIST Webbook
ripol	925.20		NIST Webbook
sg	382.67	J/molxK	NIST Webbook
sl	281.60	J/molxK	NIST Webbook
sl	280.91	J/molxK	NIST Webbook
tb	404.90	K	KDB
tc	609.00	K	KDB
tc	609.00	K	NIST Webbook
tc	606.90	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	162.00	K	Aqueous Solubility Prediction Method
tf	161.80	K	KDB
tt	161.40 ± 0.20	K	NIST Webbook
tt	161.84 ± 0.05	K	NIST Webbook
vc	0.450	m ³ /kmol	KDB
zc	0.2666120		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.88	J/molxK	448.15	NIST Webbook
cpg	152.23	J/molxK	298.15	NIST Webbook
cpg	170.36	J/molxK	323.15	NIST Webbook
cpg	197.90	J/molxK	373.15	NIST Webbook
cpg	217.63	J/molxK	408.15	NIST Webbook
cpl	214.20	J/molxK	298.15	NIST Webbook
cpl	211.79	J/molxK	298.15	NIST Webbook
dvisc	0.0014311	Paxs	258.86	Joback Method
dvisc	0.0008196	Paxs	294.64	Joback Method
dvisc	0.0029878	Paxs	223.08	Joback Method
dvisc	0.0003728	Paxs	366.21	Joback Method
dvisc	0.0002793	Paxs	401.99	Joback Method
dvisc	0.0082639	Paxs	187.30	Joback Method
dvisc	0.0005297	Paxs	330.43	Joback Method
hfust	8.28	kJ/mol	161.40	NIST Webbook
hfust	8.28	kJ/mol	161.40	NIST Webbook
hfust	8.33	kJ/mol	161.40	NIST Webbook
hfust	8.50	kJ/mol	161.50	NIST Webbook
hfust	8.33	kJ/mol	161.84	NIST Webbook
hvapt	34.04	kJ/mol	405.00	NIST Webbook
hvapt	37.90 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	38.90 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	34.31	kJ/mol	404.90	KDB
hvapt	37.00 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	38.60	kJ/mol	365.00	NIST Webbook
hvapt	36.30 ± 0.10	kJ/mol	368.00	NIST Webbook
hvapt	39.80 ± 0.10	kJ/mol	313.00	NIST Webbook
pvap	28.90	kPa	363.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K

pvap	20.40	kPa	353.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K
pvap	13.90	kPa	343.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K
pvap	40.30	kPa	373.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K
pvap	54.80	kPa	383.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K
pvap	73.20	kPa	393.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K

pvap	9.30	kPa	333.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K
pvap	3.70	kPa	313.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K
pvap	2.10	kPa	303.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K
pvap	6.00	kPa	323.15	Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K
rfi	1.42750		293.15	Density, Viscosity, Refractive Index, and Freezing Point for Binary Mixtures of 1,1'-Bicyclohexyl with Alkylcyclohexane
rfi	1.43073		298.15	KDB

rho1	779.91	kg/m3	303.15	Densities, Viscosities, Speeds of Sound, Bulk Moduli, Surface Tensions, and Flash Points of Binary Mixtures of Ethylcyclohexane or Methylcyclohexane with n-Dodecane or n-Hexadecane at 0.1 MPa
rho1	763.59	kg/m3	323.15	Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of 2,2,4-Trimethylpentane with Several Alkylated Cyclohexanes from (293.15 to 343.15) K
rho1	755.35	kg/m3	333.15	Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of 2,2,4-Trimethylpentane with Several Alkylated Cyclohexanes from (293.15 to 343.15) K
rho1	747.03	kg/m3	343.15	Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of 2,2,4-Trimethylpentane with Several Alkylated Cyclohexanes from (293.15 to 343.15) K

rho1	787.98	kg/m3	293.15	Densities, Viscosities, Speeds of Sound, Bulk Moduli, Surface Tensions, and Flash Points of Binary Mixtures of Ethylcyclohexane or Methylcyclohexane with n-Dodecane or n-Hexadecane at 0.1 MPa
rho1	767.69	kg/m3	318.15	Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of 2,2,4-Trimethylpentane with Several Alkylated Cyclohexanes from (293.15 to 343.15) K
rho1	771.79	kg/m3	313.15	Densities, Viscosities, Speeds of Sound, Bulk Moduli, Surface Tensions, and Flash Points of Binary Mixtures of Ethylcyclohexane or Methylcyclohexane with n-Dodecane or n-Hexadecane at 0.1 MPa
rho1	763.60	kg/m3	323.15	Densities, Viscosities, Speeds of Sound, Bulk Moduli, Surface Tensions, and Flash Points of Binary Mixtures of Ethylcyclohexane or Methylcyclohexane with n-Dodecane or n-Hexadecane at 0.1 MPa

rho1	755.36	kg/m3	333.15	Densities, Viscosities, Speeds of Sound, Bulk Moduli, Surface Tensions, and Flash Points of Binary Mixtures of Ethylcyclohexane or Methylcyclohexane with n-Dodecane or n-Hexadecane at 0.1 MPa
rho1	787.98	kg/m3	293.15	Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane
rho1	783.95	kg/m3	298.15	Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane
rho1	779.92	kg/m3	303.15	Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane
rho1	775.87	kg/m3	308.15	Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane
rho1	771.80	kg/m3	313.15	Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane
rho1	767.72	kg/m3	318.15	Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane

rho1	763.62	kg/m3	323.15	Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane
rho1	788.02	kg/m3	293.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes
rho1	784.01	kg/m3	298.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes
rho1	771.82	kg/m3	313.15	Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of 2,2,4-Trimethylpentane with Several Alkylated Cyclohexanes from (293.15 to 343.15) K
rho1	775.93	kg/m3	308.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes
rho1	771.86	kg/m3	313.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes

rho	767.78	kg/m ³	318.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes
rho	775.88	kg/m ³	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of 2,2,4-Trimethylpentane with Several Alkylated Cyclohexanes from (293.15 to 343.15) K
rho	779.93	kg/m ³	303.15	Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of 2,2,4-Trimethylpentane with Several Alkylated Cyclohexanes from (293.15 to 343.15) K
rho	783.97	kg/m ³	298.15	Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of 2,2,4-Trimethylpentane with Several Alkylated Cyclohexanes from (293.15 to 343.15) K
rho	787.98	kg/m ³	293.15	Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of 2,2,4-Trimethylpentane with Several Alkylated Cyclohexanes from (293.15 to 343.15) K
rho	788.00	kg/m ³	293.00	KDB

rho1	779.98	kg/m ³	303.15	Excess Molar Volume along with Viscosity and Refractive Index for Binary Systems of Tricyclo[5.2.1.0(2.6)]decane with Five Cycloalkanes
sfust	51.30	J/molxK	161.40	NIST Webbook
sfust	51.49	J/molxK	161.84	NIST Webbook
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40223e+01
Coeff. B	-3.39182e+03
Coeff. C	-4.43220e+01
Temperature range (K), min.	291.27
Temperature range (K), max.	433.70

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	7.23704e+01
Coeff. B	-7.17302e+03
Coeff. C	-8.45462e+00
Coeff. D	4.40351e-06
Temperature range (K), min.	161.84
Temperature range (K), max.	609.15

Sources

THERMODYNAMICS OF MIXTURES CONTAINING ALKOXYETHANOLS. Excess Liquid Critical Temperature of Some Alkyl Alkyls and Cyclic Hydrocarbons. K. NES, Prediction for n-Hexadecane and n-Heptane Pressure Data, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K:

<https://www.doi.org/10.1016/j.tca.2011.04.012>

<https://www.doi.org/10.1021/je0341357>

<https://www.doi.org/10.1021/acs.jced.8b00125>

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=495>

KDB: <https://www.cheric.org/files/research/kdb/mol/mol495.mol>

Liquid liquid equilibria for the binary systems of sulfolane with branched alkanes, viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Hexamethylphosphoramide (KDBs with Energy, Chemical and Physical Properties Databank): Activity coefficients at infinite dilution of organic solutes in the ionic liquid $[\text{C}_4\text{mim}][\text{PF}_6]$ by the Crippen Method: methanesulfonate; McGowan Method: <https://www.doi.org/10.1016/j.fluid.2006.05.008>
<https://www.doi.org/10.1021/acs.jced.9b00544>
<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=495>
<https://www.doi.org/10.1016/j.fluid.2010.10.008>
<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
<http://link.springer.com/article/10.1007/BF02311772>

The Yaws Handbook of Vapor Pressure: Densities, Viscosities, Speeds of Sound, Bulk Moduli, Surface Tensions, and Heat of Vaporization for the Binary Systems of Hexamethylphosphoramide with n-Alkanes: n-Dodecane or n-Hexadecane at 0.1 MPa: Solubilities of Alkylcyclohexanes in Water from 30 C to 180 C: Density, Viscosity, Refractive Index, and Freezing Point for Binary Mixtures of Thermally Stable Polymers Containing Precursors of Vitamin B5: Crippen Method: <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<https://www.doi.org/10.1021/acs.jced.8b00008>
<https://www.doi.org/10.1021/je020208v>
https://en.wikipedia.org/wiki/Joback_method
<https://www.doi.org/10.1021/je0342567>
<https://www.doi.org/10.1021/je500275j>
<https://www.doi.org/10.1021/je020060f>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Critical Point Measurements for Five n-Alkylcyclohexanes (C6 to C10) by the Pitzer Equation Method: organic interactions of volatile organic compounds with the ionic liquids $[\text{C}_4\text{mim}][\text{PF}_6]$ and $[\text{C}_4\text{mim}][\text{BF}_4]$ at infinite dilution: Density, Viscosity, Refractive Index, and Surface Tensions of Binary Mixtures of $[\text{C}_4\text{mim}][\text{PF}_6]$ with Several n-Alkylcyclohexanes from 293.15 to 343.15 K: Thermodynamic Properties of Volatile Organic Compounds with the Ionic Liquid $[\text{C}_4\text{mim}][\text{PF}_6]$: Density, Viscosity, Refractive Index, and Surface Tension for Binary Systems of the amine group at cyclohexane, n-dodecane, and n-hexadecane (with HWT) by the modified UNIFAC (Dortmund) model and validation in multicomponent systems containing cyclohexane: <https://www.doi.org/10.1021/je0256535>
<https://www.doi.org/10.1016/j.jct.2011.09.028>
<https://www.doi.org/10.1016/j.jct.2012.09.017>
<https://www.doi.org/10.1021/acs.jced.5b00105>
<https://www.doi.org/10.1016/j.jct.2013.05.035>
<https://www.doi.org/10.1021/je0502041>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1678917&Units=SI>
<https://www.doi.org/10.1021/je200822w>
<https://www.doi.org/10.1021/je400529k>
<https://www.doi.org/10.1016/j.fluid.2011.09.010>

Legend

- af: Acentric Factor
- ap: Aniline Point
- chl: Standard liquid enthalpy of combustion
- cpg: Ideal gas heat capacity
- cpl: Liquid phase heat capacity
- dm: Dipole Moment
- 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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