Cyclohexane, (1-methylethyl)-

Other names:	(1-METHYLETHYL)CYCLOHEXANE
	Cyclohexane, isopropyl-
	HEXAHYDROCUMENE
	Isopropylcyclohexane
	NORMANTHANE
	cyclohexane, 1-methylethyl-
Inchi:	InChI=1S/C9H18/c1-8(2)9-6-4-3-5-7-9/h8-9H,3-7H2,1-2H3
InchiKey:	GWESVXSMPKAFAS-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CC(C)C1CCCCC1
Mol. weight [g/mol]:	126.24
CAS:	696-29-7

Physical Properties

Property code	Value	Unit	Source
af	0.2370		KDB
ap	322.050	K	KDB
dm	0.00	debye	KDB
gf	46.91	kJ/mol	Joback Method
hcg	5885.22	kJ/mol	KDB
hcn	5488.990	kJ/mol	KDB
hf	-180.05	kJ/mol	Joback Method
hfus	7.38	kJ/mol	Joback Method
hvap	44.04	kJ/mol	NIST Webbook
ie	9.33	eV	NIST Webbook
ie	9.55 ± 0.03	eV	NIST Webbook
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2830.00	kPa	KDB
rinpol	927.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	916.90		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	917.30		NIST Webbook
rinpol	934.00		NIST Webbook

rinpol	913.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	921.20		NIST Webbook
rinpol	926.10		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	920.00		NIST Webbook
tb	427.70 ± 0.20	K	NIST Webbook
tb	427.70	K	KDB
tb	428.20	K	NIST Webbook
tb	426.65 ± 1.50	K	NIST Webbook
tb	427.45 ± 0.50	K	NIST Webbook
tb	421.65 ± 2.00	K	NIST Webbook
tb	419.00 ± 6.00	K	NIST Webbook
tb	428.15 ± 6.00	K	NIST Webbook
tb	421.65 ± 4.00	K	NIST Webbook
tb	427.90 ± 0.50	K	NIST Webbook
tb	425.50 ± 2.00	K	NIST Webbook
tb	427.65 ± 0.20	K	NIST Webbook
tb	427.65 ± 0.30	K	NIST Webbook
tb	427.55 ± 0.30	K	NIST Webbook
tb	427.15 ± 1.00	K	NIST Webbook

tb	427.80 ± 0.50	K	NIST Webbook
tb	427.71 ± 0.03	K	NIST Webbook
tb	427.72 ± 0.30	K	NIST Webbook
tb	427.71 ± 0.20	K	NIST Webbook
tb	427.00 ± 4.00	K	NIST Webbook
tc	632.20	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	640.00	K	KDB
tf	183.40	K	KDB
tf	182.75 ± 0.30	K	NIST Webbook
tf	183.35 ± 0.30	K	NIST Webbook
tf	183.35 ± 0.20	K	NIST Webbook
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.22	J/mol×K	424.43	Joback Method
cpg	274.32	J/mol×K	458.39	Joback Method
cpg	292.50	J/mol×K	492.34	Joback Method
cpg	309.76	J/mol×K	526.30	Joback Method
cpg	341.65	J/mol×K	594.22	Joback Method
cpg	356.32	J/mol×K	628.17	Joback Method
cpg	326.13	J/mol×K	560.26	Joback Method
dvisc	0.0042812	Pa×s	223.71	Joback Method
dvisc	0.0017447	Pa×s	263.86	Joback Method
dvisc	0.0155571	Pa×s	183.57	Joback Method
dvisc	0.0005431	Pa×s	344.14	Joback Method
dvisc	0.0003638	Pa×s	384.29	Joback Method
dvisc	0.0002629	Pa×s	424.43	Joback Method
dvisc	0.0009012	Pa×s	304.00	Joback Method
hvapt	44.10	kJ/mol	363.00	NIST Webbook
hvapt	41.10	kJ/mol	386.50	NIST Webbook
rfi	1.43861		298.15	KDB

rhol	794.32	kg/m3	303.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	778.64	kg/m3	323.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	774.69	kg/m3	328.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	770.73	kg/m3	333.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	766.76	kg/m3	338.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries

rhol	762.78	kg/m3	343.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	798.22	kg/m3	298.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	782.57	kg/m3	318.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	790.41	kg/m3	308.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	786.50	kg/m3	313.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries

rhol	782.57	kg/m3	318.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	778.63	kg/m3	323.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	774.69	kg/m3	328.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	770.73	kg/m3	333.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	762.78	kg/m3	343.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries

rhol	786.50	kg/m3	313.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	790.41	kg/m3	308.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	794.32	kg/m3	303.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	798.22	kg/m3	298.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries
rhol	802.11	kg/m3	293.15	Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries

rhol	762.84	kg/m3	343.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K
rhol	766.81	kg/m3	338.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K
rhol	770.77	kg/m3	333.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K
rhol	774.72	kg/m3	328.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K

rhol	778.66	kg/m3	323.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K
rhol	782.59	kg/m3	318.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K
rhol	786.51	kg/m3	313.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K
rhol	790.43	kg/m3	308.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K

rhol	794.34	kg/m3	303.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K
rhol	798.24	kg/m3	298.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K
rhol	802.14	kg/m3	293.15	Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Cyclopropanemethanol and Corresponding Binaries at T = (293.15 to 343.15) K
rhol	802.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44998e+01
Coeff. B	-3.74505e+03
Coeff. C	-4.70030e+01
Temperature range (K), min.	310.51
Temperature range (K), max.	454.59

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.16195e+01
Coeff. B	-8.01121e+03
Coeff. C	-9.76424e+00
Coeff. D	4.82817e-06
Temperature range (K), min.	183.76
Temperature range (K), max.	640.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Densities and Viscosities for the Ternary System of 1,2,3,4-Tetrahydronaphthalene + Isopropylcyclohexane + Methyl Laurate and Corresponding Binaries at T = (293.15 to 343.15) K:	https://www.doi.org/10.1021/acs.jced.8b00662
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C696297&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol560.mol
Densities and Viscosities for the Ternary Mixtures of exo-Tetrahydrodicyclopentadiene (1) + Isopropylcyclohexane (2) + Methyl Laurate (3) and Corresponding Binaries:	https://www.doi.org/10.1021/acs.jced.9b00397
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=560
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=560
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
ap:	Aniline Point
cpg:	Ideal gas 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

hfus:	Enthalpy of fusion at standard conditions
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume