1-Hexanol, 2-ethyl-

Other names:	2-EH
	2-Ethyl-1-hexanol
	2-Ethyl-1-hexyl alcohol
	2-Ethyl-hexanol-1
	2-Ethylhexan-1-ol
	2-Ethylhexanol
	2-Ethylhexyl alcohol
	Ethyl-1-hexanol,2-
	Ethylhexanol
	Ethylhexyl alcohol
	Hexan-1-ol, 2-ethyl
	Hexanol, 2-ethyl-
	NSC 9300
	OCTYL ALCOHOL
Inchi:	InChI=1S/C8H18O/c1-3-5-6-8(4-2)7-9/h8-9H,3-7H2,1-2H3
InchiKey:	YIWUKEYIRIRTPP-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCCC(CC)CO
Mol. weight [g/mol]:	130.23
CAS:	104-76-7

Physical Properties

Property code	Value	Unit	Source
chl	-5287.78 ± 0.79	kJ/mol	NIST Webbook
dm	1.80	debye	KDB
gf	-122.78	kJ/mol	Joback Method
hf	-365.50	kJ/mol	KDB
hf	-367.50 ± 2.20	kJ/mol	NIST Webbook
hfl	-432.88 ± 0.79	kJ/mol	NIST Webbook
hfus	17.04	kJ/mol	Joback Method
hvap	68.50 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.11		Estimated Solubility Method
log10ws	-2.11		Aqueous Solubility Prediction Method
logp	2.195		Crippen Method
mcvol	129.450	ml/mol	McGowan Method

nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	2800.00 ± 100.00	kPa	NIST Webbook
pc	2800.00 ± 200.00	kPa	NIST Webbook
pc	2800.00	kPa	KDB
rinpol	1038.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	164.40		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1030.00		NIST Webbook
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rinpol	1043.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1028.00		NIST Webbook
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rinpol	1008.00		NIST Webbook
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rinpol	1013.00	NIST Webbook
rinpol	1064.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1018.00	NIST Webbook
rinpol	1015.00	NIST Webbook
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rinpol	1016.10	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1048.00	NIST Webbook
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rinpol	1019.00	NIST Webbook
rinpol	1014.90	NIST Webbook
rinpol	1037.00	NIST Webbook
rinpol	1016.90	NIST Webbook
rinpol	1015.20	NIST Webbook
rinpol	1045.00	NIST Webbook
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rinpol	1026.30	NIST Webbook
rinpol	1010.70	NIST Webbook
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ripol	1484.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1503.00		NIST Webbook
sl	347.00	J/mol×K	NIST Webbook
tb	458.20	K	(Liquid + liquid) equilibria of (water + propionic acid + 2-ethyl-1-hexanol): Experimental data and correlation
tb	457.77	K	KDB
tc	640.60	K	KDB
tc	641.00 ± 1.00	K	NIST Webbook
tc	641.00 ± 2.00	K	NIST Webbook
tc	640.20 ± 0.30	K	NIST Webbook

tf	203.00	K	KDB
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.43	J/mol×K	555.64	Joback Method
cpg	313.47	J/mol×K	528.49	Joback Method
cpg	302.08	J/mol×K	501.33	Joback Method
cpg	290.23	J/mol×K	474.18	Joback Method
cpg	345.08	J/mol×K	609.94	Joback Method
cpg	334.96	J/mol×K	582.79	Joback Method
cpg	354.79	J/mol×K	637.10	Joback Method
cpl	317.50	J/mol×K	298.15	NIST Webbook
dvisc	0.1178389	Pa×s	225.74	Joback Method
dvisc	0.0001689	Pa×s	474.18	Joback Method
dvisc	0.0041171	Pa×s	308.55	Joback Method
dvisc	0.0013956	Pa×s	349.96	Joback Method
dvisc	0.0005948	Pa×s	391.37	Joback Method
dvisc	0.0002984	Pa×s	432.77	Joback Method
dvisc	0.0169844	Pa×s	267.15	Joback Method
hvapt	52.70	kJ/mol	385.50	NIST Webbook
hvapt	60.20	kJ/mol	402.00	NIST Webbook
pvap	75.01	kPa	447.04	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol
pvap	49.22	kPa	433.51	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol

pvap	55.52	kPa	437.24	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol
pvap	59.61	kPa	439.49	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol
pvap	64.64	kPa	442.12	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol
pvap	70.55	kPa	445.00	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol
pvap	45.05	kPa	430.79	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol

pvap	79.55	kPa	449.02	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol	
pvap	84.49	kPa	451.06	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol	
pvap	99.44	kPa	456.77	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol	
pvap	102.20	kPa	457.83	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol	

pvap	102.91	kPa	458.23	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol
pvap	39.67	kPa	426.95	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol
pvap	40.00	kPa	427.20	Isobaric Vapor Liquid Equilibria for Binary Systems Comprising 1-Chloro-2-ethylhexane, 2-Ethyl-1-hexanol, p-Xylene, and N-Methylpyrrolidone (NMP) at 40.0 kPa
pvap	30.03	kPa	418.24	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol
pvap	19.88	kPa	407.11	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol

pvap	9.88	kPa	389.76	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol	
pvap	0.34	kPa	331.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.28	kPa	328.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.22	kPa	325.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	

pvap	0.17	kPa	322.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.14	kPa	319.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.11	kPa	316.30	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.09	kPa	313.30	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	

pvap	0.05	kPa	307.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.04	kPa	304.50	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.03	kPa	301.60	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	
pvap	0.02	kPa	298.70	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols	

pvap	0.07	kPa	310.30	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	103.26	kPa	458.24	Vapor Liquid Equilibrium, Excess Molar Enthalpies, and Excess Molar Volumes of Binary Mixtures Containing Methyl Isobutyl Ketone (MIBK) and 2-Butanol, tert-Pentanol, or 2-Ethyl-1-hexanol
pvap	0.02	kPa	293.80	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
rfi	1.43100		293.10	Phase Equilibria of Binary Systems Comprising Formic Acid, N,N-Dimethylformamide, 1-Chloro-2-ethylhexane, and 2-Ethyl-1-hexanol
rfi	1.42920		298.15	Acoustic and Thermodynamic Properties of 2-Ethyl-1-hexanol by Means of High-Pressure Speed of Sound Measurements at Temperatures from (293 to 318) K and Pressures up to 101 MPa

rfi	1.42930		298.20	Tie-line data for the aqueous solutions of phenol with organic solvents at T = 298.2 K
rfi	1.42930		298.20	Solubility and tie line data for the aqueous solutions of butyric acid with 1-octanol and 2-ethyl-1-hexanol at various temperatures
rfi	1.43100		293.10	Vapor-Liquid Equilibria of Binary Systems Comprising 1-Chloro-2-ethylhexane and 2-Ethyl-1-hexanol
rhol	833.00	kg/m3	293.00	KDB
rhol	821.68	kg/m3	308.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Ethyl-1-hexanol with Benzene and Halobenzenes
rhol	825.39	kg/m3	303.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Ethyl-1-hexanol with Benzene and Halobenzenes
rhol	829.07	kg/m3	298.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Ethyl-1-hexanol with Benzene and Halobenzenes

speedsl	1318.07	m/s	298.15	Densities, Speeds of Sound, and Isentropic Compressibilities for Binary Mixtures of 2-Ethyl-1-hexanol with 1-Pentanol, 1-Heptanol, or 1-Nonanol at the Temperature 298.15 K
speedsl	1318.44	m/s	298.15	Densities, Speeds of Sound, and Isentropic Compressibilities for Binary Mixtures of 1,2-Ethanediol with 2-Ethyl-1-hexanol, 1-Heptanol, or Ethanol at the Temperature 298.15 K and Densities for Mixtures of 1,2-Ethanediol with 1-Nonanol at the Temperatures (293.15 and 298.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43882e+01
Coeff. B	-3.40352e+03
Coeff. C	-1.07630e+02
Temperature range (K), min.	349.00
Temperature range (K), max.	482.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.04517e+02

Coeff. B	-2.04556e+04
Coeff. C	-4.24888e+01
Coeff. D	2.42482e-05
Temperature range (K), min.	203.15
Temperature range (K), max.	640.25

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Legend

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
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume