2-Heptanol

Other names:	1-Methylhexanol
	2-Heptyl alcohol
	2-Hydroxyheptane
	Amyl methyl carbinol
	CH3(CH2)4CHOHCH3
	Heptan-2-ol
	Heptanol-2
	Methyl amyl carbinol
	NSC 2220
	amylmethylcarbinol
	methylpentylcarbinol
	n-Heptan-2-ol
	s-Heptyl alcohol
Inchi:	InChI=1S/C7H16O/c1-3-4-5-6-7(2)8/h7-8H,3-6H2,1-2H3
InchiKey:	CETWDUZRCINIHU-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCCC(C)O
Mol. weight [g/mol]:	116.20
CAS:	543-49-7

Physical Properties

Property code	Value	Unit	Source
cpl	298.64	J/mol×K	Vapour pressures and heat capacity measurements on the C7 C9 secondary aliphatic alcohols
dvisc	0.0053460	Pa×s	Speeds of sound, isentropic compressibilities, viscosities and excess molar volumes of binary mixtures of methylcyclohexane + 2-alkanols or ethanol at T = 298.15 K
gf	-131.20	kJ/mol	Joback Method
hf	-355.40 ± 2.10	kJ/mol	NIST Webbook
hfl	-416.90 ± 0.67	kJ/mol	NIST Webbook
hfus	14.45	kJ/mol	Joback Method
hvap	62.10 ± 0.40	kJ/mol	NIST Webbook

ie	10.24	eV	NIST Webbook
ie	9.70 ± 0.03	eV	NIST Webbook
log10ws	-1.55		Estimated Solubility Method
log10ws	-1.55		Aqueous Solubility Prediction Method
logp	1.948		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3021.00 ± 20.00	kPa	NIST Webbook
pc	3021.00 ± 20.00	kPa	NIST Webbook
pc	3020.00 ± 20.00	kPa	NIST Webbook
pc	3021.00	kPa	KDB
rhoc	262.61 ± 19.75	kg/m3	NIST Webbook
rhoc	262.61 ± 2.32	kg/m3	NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	882.50		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	901.40		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	900.00		NIST Webbook

rinpol	900.00	NIST Webbook
rinpol	903.00	NIST Webbook
rinpol	903.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	911.00	NIST Webbook
rinpol	885.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	915.00	NIST Webbook
rinpol	905.10	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	903.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	919.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	889.00	NIST Webbook
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rinpol	908.00	NIST Webbook
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rinpol	894.00	NIST Webbook
rinpol	875.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	918.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	904.00	NIST Webbook
rinpol	909.00	NIST Webbook
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rinpol	889.00	NIST Webbook

rinpol	896.00	NIST Webbook
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rinpol	883.00	NIST Webbook
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rinpol	886.00	NIST Webbook
rinpol	888.00	NIST Webbook
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rinpol	877.00	NIST Webbook
rinpol	868.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	888.40	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	882.30	NIST Webbook
rinpol	882.30	NIST Webbook
ripol	1285.00	NIST Webbook
ripol	1318.00	NIST Webbook
ripol	1293.00	NIST Webbook
ripol	1284.00	NIST Webbook
ripol	1320.00	NIST Webbook
ripol	1324.00	NIST Webbook
ripol	1322.00	NIST Webbook
ripol	1304.00	NIST Webbook
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ripol	1320.00	NIST Webbook
ripol	1286.00	NIST Webbook

ripol	1326.00	NIST Webbook
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ripol	1310.00	NIST Webbook
ripol	1333.00	NIST Webbook

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ripol	1324.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1316.00		NIST Webbook
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ripol	1311.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1290.00		NIST Webbook
tb	432.55 ± 1.00	K	NIST Webbook
tb	432.00	K	KDB

tb	434.20	K	NIST Webbook
tb	432.65 ± 2.00	K	NIST Webbook
tb	433.55 ± 0.50	K	NIST Webbook
tb	432.85 ± 0.50	K	NIST Webbook
tb	434.15 ± 3.00	K	NIST Webbook
tb	430.65 ± 3.00	K	NIST Webbook
tb	432.15 ± 2.00	K	NIST Webbook
tb	429.40 ± 3.00	K	NIST Webbook
tb	431.85 ± 0.50	K	NIST Webbook
tb	429.65 ± 3.00	K	NIST Webbook
tb	434.15 ± 1.00	K	NIST Webbook
tb	431.15 ± 3.00	K	NIST Webbook
tc	608.30	K	KDB
tc	608.30 ± 0.60	K	NIST Webbook
tc	608.60 ± 0.60	K	NIST Webbook
tc	608.30 ± 0.60	K	NIST Webbook
tc	608.38	K	NIST Webbook
tc	611.40 ± 0.25	K	NIST Webbook
tf	243.00	K	KDB
vc	0.442	m3/kmol	NIST Webbook
vc	0.442	m3/kmol	KDB
zc	0.2640090		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.92	J/mol×K	451.30	Joback Method
cpg	258.79	J/mol×K	478.59	Joback Method
cpg	269.25	J/mol×K	505.89	Joback Method
cpg	279.32	J/mol×K	533.18	Joback Method
cpg	289.00	J/mol×K	560.47	Joback Method
cpg	298.30	J/mol×K	587.77	Joback Method
cpg	307.23	J/mol×K	615.06	Joback Method
dvisc	0.0041520	Pa×s	303.15	Densities and viscosities of binary mixtures of ethylmethylketone and 2-alkanols; application of the ERAS model and cubic EOS

dvisc	0.0034780	Pa×s	308.15	Densities and viscosities of binary mixtures of ethylmethylketone and 2-alkanols; application of the ERAS model and cubic EOS
dvisc	0.0028530	Pa×s	313.15	Densities and viscosities of binary mixtures of ethylmethylketone and 2-alkanols; application of the ERAS model and cubic EOS
dvisc	0.0050030	Pa×s	298.15	Densities and viscosities of binary mixtures of ethylmethylketone and 2-alkanols; application of the ERAS model and cubic EOS
dvisc	0.0050230	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Cyclohexanone and 2-Alkanols
dvisc	0.0041510	Pa×s	303.15	Densities and Viscosities of Binary Mixtures of Cyclohexanone and 2-Alkanols
dvisc	0.0034780	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Cyclohexanone and 2-Alkanols
dvisc	0.0028520	Pa×s	313.15	Densities and Viscosities of Binary Mixtures of Cyclohexanone and 2-Alkanols
hvapt	59.80	kJ/mol	378.00	NIST Webbook
hvapt	54.40	kJ/mol	392.00	NIST Webbook
hvapt	51.60	kJ/mol	394.00	NIST Webbook
hvapt	66.10	kJ/mol	291.00	NIST Webbook

rfi	1.41880	298.15	Densities, Viscosities, and Refractive Indices of Binary Mixtures of Acetophenone and 2-Alkanols	
rfi	1.42060	293.15	Densities, viscosities, excess molar volumes, and refractive indices of acetonitrile and 2-alkanols binary mixtures at different temperatures: Experimental results and application of the Prigogine Flory Patterson theory	
rfi	1.41880	298.15	Densities, viscosities, excess molar volumes, and refractive indices of acetonitrile and 2-alkanols binary mixtures at different temperatures: Experimental results and application of the Prigogine Flory Patterson theory	
rfi	1.41650	303.15	Densities, viscosities, excess molar volumes, and refractive indices of acetonitrile and 2-alkanols binary mixtures at different temperatures: Experimental results and application of the Prigogine Flory Patterson theory	

rfi	1.41430		308.15	Densities, viscosities, excess molar volumes, and refractive indices of acetonitrile and 2-alkanols binary mixtures at different temperatures: Experimental results and application of the Prigogine Flory Patterson theory
rhol	797.65	kg/m3	318.15	The study of physico-chemical properties of binary systems consisting of N-Methylcyclohexylamine with 2-alkanols at T = (298.15-328.15) K
rhol	813.36	kg/m3	298.15	The study of physico-chemical properties of binary systems consisting of N-Methylcyclohexylamine with 2-alkanols at T = (298.15-328.15) K
rhol	801.46	kg/m3	313.15	Densities and viscosities of the mixtures (formamide + 2-alkanol): Experimental and theoretical approaches
rhol	805.72	kg/m3	308.15	Densities and viscosities of the mixtures (formamide + 2-alkanol): Experimental and theoretical approaches
rhol	809.50	kg/m3	303.15	Densities and viscosities of the mixtures (formamide + 2-alkanol): Experimental and theoretical approaches

rhol	813.38	kg/m3	298.15	Densities and viscosities of the mixtures (formamide + 2-alkanol): Experimental and theoretical approaches
rhol	813.74	kg/m3	298.15	Study of thermodynamic and transport properties of binary liquid mixtures of n-decane with hexan-2-ol, heptan-2-ol and octan-2-ol at T = 298.15 K. Experimental results and application of the Prigogine-Flory-Patterson theory
rhol	804.88	kg/m3	308.15	Densities, viscosities and ultrasonic velocities of binary mixtures of methylbenzene with hexan-2-ol, heptan-2-ol and octan-2-ol at T = 298.15 and 308.15K
rhol	813.74	kg/m3	298.15	Densities, viscosities and ultrasonic velocities of binary mixtures of methylbenzene with hexan-2-ol, heptan-2-ol and octan-2-ol at T = 298.15 and 308.15K
rhol	805.72	kg/m3	308.15	The study of physico-chemical properties of binary systems consisting of N-Methylcyclohexylamine with 2-alkanols at T = (298.15-328.15) K

rhol	801.50	kg/m3	313.15	Thermodynamic Properties of Binary Mixtures Containing N,N-Dimethylacetamide + 2-Alkanol: Experimental Data and Modeling
rhol	805.70	kg/m3	308.15	Thermodynamic Properties of Binary Mixtures Containing N,N-Dimethylacetamide + 2-Alkanol: Experimental Data and Modeling
rhol	809.50	kg/m3	303.15	Thermodynamic Properties of Binary Mixtures Containing N,N-Dimethylacetamide + 2-Alkanol: Experimental Data and Modeling
rhol	813.20	kg/m3	298.15	Thermodynamic Properties of Binary Mixtures Containing N,N-Dimethylacetamide + 2-Alkanol: Experimental Data and Modeling
rhol	789.38	kg/m3	328.15	The study of physico-chemical properties of binary systems consisting of N-Methylcyclohexylamine with 2-alkanols at T = (298.15-328.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38938e+01
Coeff. B	-2.80782e+03
Coeff. C	-1.29285e+02

Temperature range (K), min.	335.65
Temperature range (K), max.	456.45

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.14758e+02
Coeff. B	-1.04894e+04
Coeff. C	-1.44255e+01
Coeff. D	8.88948e-06
Temperature range (K), min.	243.00
Temperature range (K), max.	588.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
313.16	1003.00	802.5
313.16	2005.00	803.3
313.16	3002.00	804.0
313.16	4013.00	804.8
313.16	5001.00	805.5
313.16	5991.00	806.2
313.16	6993.00	806.9
313.16	7994.00	807.7
313.16	9011.00	808.4
313.16	9995.00	809.1
313.16	10990.00	809.8
313.16	11988.00	810.5
313.16	13003.00	811.2
313.16	13988.00	811.9
313.16	14992.00	812.6
313.16	15990.00	813.2
313.16	17012.00	813.9
313.16	17987.00	814.5
313.16	18982.00	815.2
313.16	20004.00	815.9

313.16	20996.00	816.5
313.16	21989.00	817.2
323.09	1026.00	794.4
323.09	2006.00	795.2
323.09	3018.00	796.0
323.09	4017.00	796.8
323.09	5005.00	797.5
323.09	6018.00	798.3
323.09	7002.00	799.1
323.09	8003.00	799.8
323.09	9017.00	800.6
323.09	10017.00	801.3
323.09	10994.00	802.0
323.09	11998.00	802.8
323.09	13028.00	803.5
323.09	13997.00	804.2
323.09	15005.00	804.9
323.09	16003.00	805.6
323.09	17013.00	806.3
323.09	18009.00	807.0
323.09	19003.00	807.6
323.09	20006.00	808.3
323.09	20998.00	808.9
323.09	22011.00	809.6
333.05	1047.00	786.1
333.05	2009.00	787.0
333.05	3005.00	787.8
333.05	4010.00	788.7
333.05	5015.00	789.5
333.05	6018.00	790.3
333.05	7022.00	791.1
333.05	8012.00	791.9
333.05	9031.00	792.8
333.05	10017.00	793.5
333.05	11080.00	794.3
333.05	12039.00	795.1
333.05	13026.00	795.8
333.05	14017.00	796.6
333.05	15024.00	797.3
333.05	16018.00	798.1
333.05	17020.00	798.8
333.05	18019.00	799.5
333.05	19029.00	800.2
333.05	20016.00	800.9

333.05	21037.00	801.7
333.05	22015.00	802.4
342.96	971.00	777.4
342.96	2038.00	778.5
342.96	3013.00	779.3
342.96	4034.00	780.2
342.96	5024.00	781.1
342.96	6033.00	782.0
342.96	7015.00	782.9
342.96	8023.00	783.8
342.96	9025.00	784.7
342.96	10020.00	785.4
342.96	11029.00	786.3
342.96	12020.00	787.1
342.96	13030.00	787.9
342.96	14039.00	788.7
342.96	15023.00	789.5
342.96	16026.00	790.3
342.96	17026.00	791.1
342.96	18034.00	791.9
342.96	19026.00	792.7
342.96	20040.00	793.5
342.96	21031.00	794.2
342.96	22028.00	795.0
352.85	1038.00	769.0
352.85	2045.00	770.0
352.85	3019.00	770.9
352.85	4058.00	771.9
352.85	5028.00	772.8
352.85	6028.00	773.7
352.85	7037.00	774.7
352.85	8022.00	775.5
352.85	9078.00	776.5
352.85	10037.00	777.3
352.85	11042.00	778.2
352.85	12042.00	779.0
352.85	13042.00	779.9
352.85	14040.00	780.8
352.85	15042.00	781.6
352.85	16053.00	782.5
352.85	17058.00	783.3
352.85	18042.00	784.1
352.85	19040.00	784.9
352.85	20070.00	785.7

352.85	21055.00	786.5
352.85	22050.00	787.3
362.72	1043.00	760.1
362.72	2049.00	761.2
362.72	3066.00	762.2
362.72	4062.00	763.2
362.72	5041.00	764.2
362.72	6045.00	765.2
362.72	7046.00	766.2
362.72	8042.00	767.2
362.72	9058.00	768.1
362.72	10038.00	769.0
362.72	11054.00	770.0
362.72	12046.00	770.9
362.72	13054.00	771.8
362.72	14048.00	772.7
362.72	15049.00	773.6
362.72	16050.00	774.5
362.72	17070.00	775.4
362.72	18065.00	776.2
362.72	19060.00	777.1
362.72	20081.00	777.9
362.72	21068.00	778.8
362.72	22063.00	779.6

Reference *https://www.doi.org/10.1016/j.jct.2007.05.007*

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=839
Speeds of sound, isentropic compressibilities, viscosities and excess molar volumes of binary mixtures of methylcyclohexane + 2-alkanols (C4 to C8) at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.04.019
Study of thermodynamic and transport properties of binary liquid mixtures of cyclohexanone with 2-alkanols (C4 to C8) at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2013.05.014
Densities, viscosities, sonic velocities, molar volumes, and refractive indices of (cyclohexanone + 2-propanol and cyclohexanone + 2-butanol) at T = 298.15 K:	https://www.doi.org/10.1016/j.tca.2009.06.015
KDB Vapor Pressure Data: Experimental results and application of the Prigogine Flory Patterson theory:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=839
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility