1-Undecanol

Other names:	1-HENDECANOL
	1-Undecyl alcohol
	Alcohol c-11
	Decyl carbinol
	HENDECANOIC ALCOHOL
	Hendecyl alcohol
	N-UNDECYL ALCOHOL
	NSC 403667
	Neodol 1
	Tip-Nip
	Undecan-1-ol
	Undecanol
	Undecanol-(1)
	Undecyl alcohol
	n-Hendecylenic alcohol
	n-Undecan-1-ol
	n-Undecanol
Inchi:	InChI=1S/C11H24O/c1-2-3-4-5-6-7-8-9-10-11-12/h12H,2-11H2,1H3
InchiKey:	KJIOQYGWTQBHNH-UHFFFAOYSA-N
Formula:	C11H24O
SMILES:	CCCCCCCCCCCO
Mol. weight [g/mol]:	172.31
CAS:	112-42-5

Physical Properties

Property code	Value	Unit	Source
af	0.9400		KDB
chl	-7253.70 ± 0.80	kJ/mol	NIST Webbook
gf	-95.08	kJ/mol	Joback Method
hf	-422.60	kJ/mol	Joback Method
hfl	-504.90 ± 0.80	kJ/mol	NIST Webbook
hfus	28.33	kJ/mol	Joback Method
hvap	85.80 ± 2.10	kJ/mol	NIST Webbook
hvap	86.80	kJ/mol	NIST Webbook
hvap	85.60	kJ/mol	NIST Webbook
hvap	84.70	kJ/mol	NIST Webbook
hvap	83.50	kJ/mol	NIST Webbook

log10ws	-3.69		Crippen Method
logp	3.509		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2147.00	kPa	KDB
pc	2150.00 ± 50.00	kPa	NIST Webbook
pc	2147.00 ± 30.00	kPa	NIST Webbook
pc	2147.00 ± 30.00	kPa	NIST Webbook
rhoc	239.51	kg/m3	NIST Webbook
rhoc	239.51 ± 5.17	kg/m3	NIST Webbook
rhoc	239.51 ± 8.62	kg/m3	NIST Webbook
rinpol	1371.50		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1364.60		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1374.40		NIST Webbook
rinpol	1377.50		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1376.00		NIST Webbook

rinpol	1374.00	NIST Webbook
rinpol	1364.00	NIST Webbook
rinpol	1363.00	NIST Webbook
rinpol	1367.00	NIST Webbook
rinpol	1363.00	NIST Webbook
rinpol	1371.00	NIST Webbook
rinpol	1357.00	NIST Webbook
rinpol	1356.00	NIST Webbook
rinpol	1372.00	NIST Webbook
rinpol	1372.00	NIST Webbook
rinpol	1374.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1351.00	NIST Webbook
rinpol	1367.00	NIST Webbook
rinpol	1381.00	NIST Webbook
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rinpol	1355.00	NIST Webbook
rinpol	1368.00	NIST Webbook
rinpol	1367.00	NIST Webbook
rinpol	1357.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1382.00	NIST Webbook
rinpol	1387.00	NIST Webbook
rinpol	1356.00	NIST Webbook
rinpol	1357.00	NIST Webbook
rinpol	1358.00	NIST Webbook
rinpol	1386.00	NIST Webbook
rinpol	1370.00	NIST Webbook
rinpol	1382.00	NIST Webbook
rinpol	1364.00	NIST Webbook
rinpol	1349.00	NIST Webbook
rinpol	1361.00	NIST Webbook
rinpol	233.42	NIST Webbook
rinpol	234.77	NIST Webbook
rinpol	234.41	NIST Webbook
rinpol	1356.40	NIST Webbook
rinpol	1380.40	NIST Webbook

rinpol	1364.30		NIST Webbook
rinpol	1363.30		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1370.50		NIST Webbook
rinpol	1359.91		NIST Webbook
rinpol	1355.10		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1373.70		NIST Webbook
ripol	1861.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1883.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1827.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1867.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1840.00		NIST Webbook
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ripol	1850.00		NIST Webbook
ripol	1826.00		NIST Webbook
ripol	1886.00		NIST Webbook
ripol	1861.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1847.00		NIST Webbook
ripol	1875.00		NIST Webbook
tb	516.20	K	KDB
tb	518.30	K	Ternary liquid-liquid phase equilibria of (water-carboxylic acid-1-undecanol) systems at 298.15 K
tc	703.60	K	KDB
tf	288.45 ± 0.50	K	NIST Webbook

tf	289.63	K	Experimental (Solid + Liquid) and (Liquid + Liquid) Equilibria and Excess Molar Volume of Alkanol + Acetonitrile, Propanenitrile, and Butanenitrile Mixtures
tf	292.00	K	KDB
tf	289.65 ± 0.30	K	NIST Webbook
vc	0.718	m3/kmol	NIST Webbook
vc	0.718	m3/kmol	KDB
zc	0.2635080		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.92	J/mol×K	622.27	Joback Method
cpg	442.60	J/mol×K	569.60	Joback Method
cpg	456.02	J/mol×K	595.94	Joback Method
cpg	504.67	J/mol×K	701.29	Joback Method
cpg	493.24	J/mol×K	674.95	Joback Method
cpg	481.33	J/mol×K	648.61	Joback Method
cpg	428.64	J/mol×K	543.26	Joback Method
cpl	406.34	J/mol×K	298.15	NIST Webbook
cpl	406.80	J/mol×K	303.15	NIST Webbook
cpl	419.80	J/mol×K	303.00	NIST Webbook
cpl	414.80	J/mol×K	303.65	NIST Webbook
dvisc	0.0140250	Pa×s	298.15	Densities and Kinematic Viscosities of Ten Binary 1-Alkanol Liquid Systems at Temperatures of (293.15 and 298.15) K
dvisc	0.0172840	Pa×s	293.15	Measurement of Density and Viscosity of Binary 1-Alkanol Systems (C8-C11) at 101 kPa and Temperatures from (283.15 to 313.15) K

dvisc	0.0137210	Pa×s	298.15	Measurement of Density and Viscosity of Binary 1-Alkanol Systems (C8-C11) at 101 kPa and Temperatures from (283.15 to 313.15) K
dvisc	0.0115240	Pa×s	303.15	Measurement of Density and Viscosity of Binary 1-Alkanol Systems (C8-C11) at 101 kPa and Temperatures from (283.15 to 313.15) K
dvisc	0.0093500	Pa×s	308.15	Measurement of Density and Viscosity of Binary 1-Alkanol Systems (C8-C11) at 101 kPa and Temperatures from (283.15 to 313.15) K
dvisc	0.0171820	Pa×s	293.15	Densities and Kinematic Viscosities of Ten Binary 1-Alkanol Liquid Systems at Temperatures of (293.15 and 298.15) K
dvisc	0.0078410	Pa×s	313.15	Measurement of Density and Viscosity of Binary 1-Alkanol Systems (C8-C11) at 101 kPa and Temperatures from (283.15 to 313.15) K
hvapt	79.50	kJ/mol	333.50	NIST Webbook
hvapt	83.60	kJ/mol	317.50	NIST Webbook
hvapt	68.70	kJ/mol	458.00	NIST Webbook
hvapt	68.50	kJ/mol	463.50	NIST Webbook
hvapt	72.30	kJ/mol	454.50	NIST Webbook

rhol	829.34	kg/m3	298.15	Experimental Solid + Liquid Equilibria and Excess Molar Volume of Alkanol + Octylamine Mixtures. Analysis in Terms of ERAS, DISQUAC, and Modified UNIFAC
rhol	800.20	kg/m3	338.15	Viscosities and Densities of Fatty Alcohol Mixtures from 298.15 to 338.15 K: Estimation by Kay's Rule and Prediction by the UNIFAC-VISCO and GC-UNIMOD Group Contribution Methods
rhol	807.20	kg/m3	328.15	Viscosities and Densities of Fatty Alcohol Mixtures from 298.15 to 338.15 K: Estimation by Kay's Rule and Prediction by the UNIFAC-VISCO and GC-UNIMOD Group Contribution Methods
rhol	814.20	kg/m3	318.15	Viscosities and Densities of Fatty Alcohol Mixtures from 298.15 to 338.15 K: Estimation by Kay's Rule and Prediction by the UNIFAC-VISCO and GC-UNIMOD Group Contribution Methods
rhol	821.00	kg/m3	308.15	Viscosities and Densities of Fatty Alcohol Mixtures from 298.15 to 338.15 K: Estimation by Kay's Rule and Prediction by the UNIFAC-VISCO and GC-UNIMOD Group Contribution Methods

rhol	828.00	kg/m3	298.15	Viscosities and Densities of Fatty Alcohol Mixtures from 298.15 to 338.15 K: Estimation by Kay's Rule and Prediction by the UNIFAC-VISCO and GC-UNIMOD Group Contribution Methods

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.20	K	4.00	NIST Webbook
tbrp	404.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.77538e+01
Coeff. B	-5.52497e+03
Coeff. C	-8.51960e+01
Temperature range (K), min.	401.52
Temperature range (K), max.	529.24

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.67298e+02
Coeff. B	-2.08778e+04
Coeff. C	-3.62321e+01
Coeff. D	1.52436e-05
Temperature range (K), min.	289.05
Temperature range (K), max.	704.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	827.7
298.15	1000.00	828.2
298.15	5000.00	830.7
298.15	10000.00	833.6
298.15	15000.00	836.4
298.15	20000.00	839.2
298.15	25000.00	841.8
298.15	30000.00	844.4
298.15	35000.00	846.9
298.15	40000.00	849.4
298.15	45000.00	851.8
298.15	50000.00	854.2
298.15	55000.00	856.5
298.15	60000.00	858.7
308.15	100.00	820.9
308.15	1000.00	821.5
308.15	5000.00	824.0
308.15	10000.00	827.1
308.15	15000.00	830.0
308.15	20000.00	832.9
308.15	25000.00	835.6
308.15	30000.00	838.3
308.15	35000.00	840.9
308.15	40000.00	843.4
308.15	45000.00	845.9
308.15	50000.00	848.3
308.15	55000.00	850.7
308.15	60000.00	852.9
318.15	100.00	814.1
318.15	1000.00	814.7
318.15	5000.00	817.4
318.15	10000.00	820.6
318.15	15000.00	823.7

318.15	20000.00	826.6
318.15	25000.00	829.5
318.15	30000.00	832.3
318.15	35000.00	834.8
318.15	40000.00	837.6
318.15	45000.00	840.1
318.15	50000.00	842.6
318.15	55000.00	845.1
318.15	60000.00	847.3
328.15	100.00	807.4
328.15	1000.00	808.0
328.15	5000.00	810.8
328.15	10000.00	814.1
328.15	15000.00	817.3
328.15	20000.00	820.4
328.15	25000.00	823.3
328.15	30000.00	826.2
328.15	35000.00	829.0
328.15	40000.00	831.7
328.15	45000.00	834.4
328.15	50000.00	837.0
328.15	55000.00	839.5
328.15	60000.00	841.8
338.15	100.00	800.5
338.15	1000.00	801.1
338.15	5000.00	803.9
338.15	10000.00	807.3
338.15	15000.00	810.6
338.15	20000.00	813.8
338.15	25000.00	816.9
338.15	30000.00	819.9
338.15	35000.00	822.8
338.15	40000.00	825.6
338.15	45000.00	828.4
338.15	50000.00	831.0
338.15	55000.00	833.6
338.15	60000.00	836.0
348.15	100.00	793.3
348.15	1000.00	793.8
348.15	5000.00	797.1
348.15	10000.00	800.8
348.15	15000.00	804.3
348.15	20000.00	807.6
348.15	25000.00	810.8

348.15	30000.00	813.9
348.15	35000.00	816.9
348.15	40000.00	819.9
348.15	45000.00	822.7
348.15	50000.00	825.5
348.15	55000.00	828.1
348.15	60000.00	830.7
358.15	100.00	786.0
358.15	1000.00	786.8
358.15	5000.00	790.0
358.15	10000.00	793.9
358.15	15000.00	797.6
358.15	20000.00	801.1
358.15	25000.00	804.4
358.15	30000.00	807.7
358.15	35000.00	810.8
358.15	40000.00	813.9
358.15	45000.00	816.6
358.15	50000.00	819.6
358.15	55000.00	822.4
358.15	60000.00	824.9

Reference *https://www.doi.org/10.1016/j.jct.2011.10.023*

Sources

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Joback Method: https://en.wikipedia.org/wiki/Joback_method

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Experimental (Solid + Liquid) and (Liquid + Liquid) Equilibria and Excess Molar Volumes and Derived Properties of Liquid Butanenitrile + Propanenitrile Mixtures: https://www.doi.org/10.1021/je050262m

McGowan Method: https://www.doi.org/10.1016/j.jct.2011.10.023

Ternary liquid-liquid phase equilibria of (water-carboxylic acid-1-undecanol) systems at 298.15 K: http://link.springer.com/article/10.1007/BF02311772

Liquid Liquid Phase Behavior of Solutions of 1-Octyl- and 1-Decyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)amide (C8mim/NTf2) in n-Alkyl Alcohols, with 1-Hexanol and 1-Octanol: https://www.doi.org/10.1021/je900988a

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Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Influence of the Temperature on the Liquid Liquid Solid Equilibria of the Water + Ethanol + 1-Undecanol Ternary System:	https://www.doi.org/10.1021/acs.jced.5b00206

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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