1-Dodecanol

Other names:

1-Dodecyl Alcohol
1-Hydroxydodecane
Adol 10
Adol 12
Alcohol C-12
Alfol 12
CO-1214
CO-1214N
CO-1214S
Cachalot l-50
Cachalot l-90
Conol 20P
Conol 20PP
DUODECYL ALCOHOL
Dodecan-1-ol
Dodecanol
Dodecanol-1
Dodecyl alcohol
Dytol J-68
Epal 12
Hainol 12SS
Hydroxydodecane
Karukoru 20
LAURIC ALCOHOL
Laurinic alcohol
Lauryl 24
Lauryl alcohol
Lorol 11
Lorol 5
Lorol 7
Lorol C12
MA-1214
N-DODECYL ALCOHOL
NAA 42
Nacol 12-96
Pisol
S 1298
Sipol L12
Siponol 25
Siponol L2

	Siponol L5
	Undecyl carbinol
	n-Dodecan-1-ol
	n-Dodecanol
	n-Lauryl alcohol
	n-Lauryl alcohol, primary
Inchi:	InChI=1S/C12H26O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h13H,2-12H2,1H3
InchiKey:	LQZZUXJYWNFBMV-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CCCCCCCCCCCCO
Mol. weight [g/mol]:	186.33
CAS:	112-53-8

Physical Properties

Property code	Value	Unit	Source
chl	-7909.40 ± 0.80	kJ/mol	NIST Webbook
chl	-7950.00 ± 10.00	kJ/mol	NIST Webbook
dm	1.60	debye	KDB
gf	-87.13	kJ/mol	KDB
hf	-436.50 ± 1.00	kJ/mol	NIST Webbook
hf	-443.10	kJ/mol	KDB
hf	-436.50 ± 1.00	kJ/mol	NIST Webbook
hfl	-528.50 ± 0.80	kJ/mol	NIST Webbook
hfus	90.80	kJ/mol	Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7-, and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T) 298.15 K by Correlation Gas Chromatography
hfus	40.31	kJ/mol	Heat capacities and derived thermodynamic functions of 1-dodecanol and 1-tridecanol between 10 K and 370 K and heat capacities of 1-pentadecanol and 1-heptadecanol between 300 K and 380 K and correlationos for the heat capacity and the entropy of liquid n-alcohols

hfus	40.20	kJ/mol	Solid-Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry
hfus	37.74	kJ/mol	Measurements, Correlations, and Mod. UNIFAC (Do) Prediction of (Solid-Liquid) Phase Equilibria Diagrams in Binary Systems (Aliphatic Ketone + an Alcohol)
hsub	129.30	kJ/mol	NIST Webbook
hvap	58.98	kJ/mol	Joback Method
log10ws	-4.67		Aqueous Solubility Prediction Method
log10ws	-4.80		Estimated Solubility Method
logp	3.900		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
pc	1994.00 ± 50.00	kPa	NIST Webbook
pc	1994.00	kPa	KDB
pc	1990.00 ± 50.00	kPa	NIST Webbook
pc	1994.00 ± 50.00	kPa	NIST Webbook
pt	9.60e-05 ± 2.70e-05	kPa	NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	251.68		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	252.06		NIST Webbook
rinpol	250.63		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1458.00		NIST Webbook
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rinpol	1473.00	NIST Webbook
ripol	1950.00	NIST Webbook
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ripol	1946.00	NIST Webbook
ripol	1956.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1925.00	NIST Webbook
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ripol	1950.00		NIST Webbook
ripol	1979.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1940.00		NIST Webbook
tb	534.20	K	NIST Webbook
tb	532.50	K	(Liquid + liquid) equilibria of (water + propionic acid + alcohol) ternary systems
tb	532.00	K	KDB
tc	719.40 ± 0.80	K	NIST Webbook
tc	719.40	K	NIST Webbook
tc	719.40 ± 1.50	K	NIST Webbook
tc	719.40	K	KDB
tc	719.40 ± 0.80	K	NIST Webbook
tf	296.90	K	High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol
tf	297.22	K	Thermodynamics of organic mixtures containing amines. VIII. Systems with quinoline

tf	297.78	K	Solid-liquid phase equilibrium diagrams of binary mixtures containing fatty acids, fatty alcohol compounds and tripalmitin using differential scanning calorimetry
tf	297.65	K	Aqueous Solubility Prediction Method
tf	297.00	K	KDB
tf	296.51	K	Solid-Liquid Equilibria in Three Binary Mixtures Containing Diphenyl Carbonate
tf	296.15	K	The manufacture of organic carbonate-poly(methyl ethylacrylate) nanowebs with thermal buffering effect
tt	296.95 ± 0.50	K	NIST Webbook
vc	0.718	m3/kmol	KDB
zc	0.2393550		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.99	J/mol×K	723.91	Joback Method
cpg	493.02	J/mol×K	592.43	Joback Method
cpg	507.08	J/mol×K	618.73	Joback Method
cpg	546.03	J/mol×K	697.61	Joback Method
cpg	533.57	J/mol×K	671.32	Joback Method
cpg	520.59	J/mol×K	645.02	Joback Method
cpg	478.39	J/mol×K	566.14	Joback Method
cpl	438.42	J/mol×K	298.15	NIST Webbook
cpl	462.00	J/mol×K	316.00	NIST Webbook
cpl	439.40	J/mol×K	303.15	NIST Webbook
dvisc	0.0005414	Pa×s	425.98	Joback Method
dvisc	0.0002601	Pa×s	472.70	Joback Method
dvisc	0.0043527	Pa×s	332.54	Joback Method
dvisc	0.0000863	Pa×s	566.14	Joback Method
dvisc	0.0205746	Pa×s	285.82	Joback Method
dvisc	0.0001425	Pa×s	519.42	Joback Method
dvisc	0.0013501	Pa×s	379.26	Joback Method
hfust	40.17	kJ/mol	300.20	NIST Webbook
hfust	40.17	kJ/mol	300.20	NIST Webbook

hfust	40.31	kJ/mol	297.30	NIST Webbook
hsubt	130.10 ± 1.20	kJ/mol	289.50	NIST Webbook
hvapt	80.50	kJ/mol	358.00	NIST Webbook
hvapt	83.30	kJ/mol	333.00	NIST Webbook
hvapt	84.70 ± 0.50	kJ/mol	343.00	NIST Webbook
hvapt	73.80	kJ/mol	410.50	NIST Webbook
hvapt	67.60	kJ/mol	449.00	NIST Webbook
hvapt	71.50	kJ/mol	469.00	NIST Webbook
hvapt	95.00 ± 2.00	kJ/mol	297.00	NIST Webbook
hvapt	95.40	kJ/mol	305.00	NIST Webbook
hvapt	67.60	kJ/mol	449.00	NIST Webbook
hvapt	66.70	kJ/mol	487.50	NIST Webbook
hvapt	67.70	kJ/mol	533.10	KDB
hvapt	84.76	kJ/mol	343.15	NIST Webbook
hvapt	85.80	kJ/mol	325.50	NIST Webbook
hvapt	57.10	kJ/mol	527.50	NIST Webbook
hvapt	92.50	kJ/mol	330.00	NIST Webbook
rfi	1.44058		298.15	Liquid Liquid Phase Equilibria of 1-Propanol + Water + n-Alcohol Ternary Systems at 298.15 K and Atmospheric Pressure
rfi	1.39640		298.20	(Liquid + liquid) equilibria of the (water + butyric acid + dodecanol) ternary system
rfi	1.44120		298.20	Solubility and Tie Line Data of the Water - Phosphoric Acid Solvents at T = (303.2 and 313.2) K: An Experimental and Correlational Study
rhol	809.10	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	829.60	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
rhol	823.35	kg/m3	298.15	Phase behaviour of ionic liquid 1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate with alcohols, water and aromatic hydrocarbons
rhol	830.37	kg/m3	298.15	Liquid-liquid equilibria for aqueous sulfuric acid solutions with undecane, dodecane, or 1-dodecanol, trioctylamine or tributyl phosphate and excess and deviation properties for sub-binary systems at 298.15 K
rhol	835.00	kg/m3	293.00	KDB
rhol	816.00	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	830.90	kg/m3	298.15	Solid Liquid Equilibria, Excess Molar Volumes, and Deviations in the Molar Refractivity for the Binary Systems of Alamine 304-1 + Decane, Dodecane, or Dodecanol

rhol	802.10	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	822.80	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
svapt	246.74	J/mol×K	343.15	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66246e+01
Coeff. B	-5.32811e+03
Coeff. C	-9.04220e+01
Temperature range (K), min.	416.56
Temperature range (K), max.	561.39

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.84704e+02
Coeff. B	-2.24029e+04
Coeff. C	-3.86309e+01
Coeff. D	1.56516e-05
Temperature range (K), min.	296.95
Temperature range (K), max.	721.00

Sources

The solid-liquid phase diagrams of binary mixtures of even saturated fatty alcohols:	https://www.doi.org/10.1016/j.fluid.2011.01.028
Solid–Liquid Equilibria in Three Binary Mixtures Containing Diphenyl Carbonate:	https://www.doi.org/10.1021/je101199g
Liquid–Liquid Phase Equilibria of 1-Propanol + Water + n-Alcohol Ternary Systems at 298.15 K and Atmospheric Pressure:	https://www.doi.org/10.1021/je2002539
Solid–Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry:	https://www.doi.org/10.1021/acs.jced.8b01006
Liquid–Liquid Phase Behavior of Solutions of 1-Hexyl-3-methylimidazolium Bis((trifluoromethyl)sulfonyl)amide (C6mimNTf2) in n-Alkyl Alcohols:	https://www.doi.org/10.1021/je1011357
Solubility Determination and Correlation of ... tetrahydro-2H-pyran-2,3,4, ... Fatty Alcohol:	https://www.doi.org/10.1021/je4011097
Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7-, and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T = 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0503857
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112538&Units=SI
(Liquid + liquid) equilibria of (water + propionic acid + alcohol) ternary systems:	https://www.doi.org/10.1016/j.jct.2006.05.001
The influence of temperature on the liquid–liquid–solid equilibria of the ternary system water + ethanol + 1-dodecanol:	https://www.doi.org/10.1016/j.fluid.2005.06.027
Water–Phosphoric Acid Solvents at T (303.2 and 313.2) K: An Experimental and Correlational Study:	https://www.doi.org/10.1016/j.tca.2013.02.006
Phase behaviour of ionic liquid 1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate with alcohols, water and aromatic hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2013.01.027
High Pressure Phase Behavior of the Homologous Series CO2 + 1-Alcohols:	https://www.doi.org/10.1021/acs.jced.7b01000
Experimental Measurement and Thermodynamic Model of Liquid-Liquid Equilibrium for the Ternary System of 1-Dodecanol-Phenol-Water:	https://www.doi.org/10.1021/acs.jced.9b00176
Thermophysical properties and thermodynamic phase behavior of ionic liquids:	https://www.doi.org/10.1016/j.tca.2006.06.018
Liquid Viscosity and Interfacial Tension of Binary and Ternary Mixtures Containing n-Octacosane by Surface Light Scattering:	https://www.doi.org/10.1021/acs.jced.8b01139
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Phase behavior of the carbon dioxide p 1-dodecanol system at high pressures:	https://www.doi.org/10.1016/j.fluid.2016.06.014
Thermodynamics of organic mixtures containing amines. VIII. Systems with quinoline:	https://www.doi.org/10.1016/j.jct.2008.03.015
Measurements, Correlations, and Mod. UNIFAC (Do) Prediction of (Solid-Liquid) Phase Equilibria Diagrams in Binary Systems (Aliphatic Ketone + an Alcohol):	https://www.doi.org/10.1021/je100725a
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=852
Liquid-Liquid Phase Behavior of Solutions of 1-Octyl- and 1-Decyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide (C8,10mimNTf2) in n-Alkyl Alcohols:	https://www.doi.org/10.1021/je900988a
Solvent Polarity Effect when Amberlite LA2 Is Used in the Extraction of Picric Acid:	https://www.doi.org/10.1021/acs.jced.6b00970
The manufacture of organic carbonate-poly(methyl ethylacrylate) nanowebs with thermal buffering effect:	https://www.doi.org/10.1016/j.tca.2017.10.003
Heat capacities and derived thermodynamic functions of 1-dodecanol and 1-tridecanol between 10 K and 370 K and heat capacities of 1-pentadecanol and 1-heptadecanol between 300 K and 380 K and correlations for the heat capacity and the entropy of liquid n-alcohols:	https://www.doi.org/10.1021/je025524o
Density-Pressure Relationship in Hydrogen-Bonded Mixtures: 1,4-Butanediol + 1-Dodecanol:	https://www.doi.org/10.1021/je049663c
Liquid-Liquid Phase Behavior of Solutions of 1-Dodecyl-3-methylimidazolium Bis(trifluoromethylsulphonyl)imide (C12mimNTf2) in n-Alkyl Alcohols:	https://www.doi.org/10.1021/je100359x
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Vapor-Liquid Equilibria of Binary Systems of Ethene Oxide + Dodecane, Ethene Oxide + 1-Decanol, and Ethene Oxide + 1-Dodecanol and Prediction with the Predictive Soave-Redlich-Kwong (PSRK) Equation of State:	https://www.doi.org/10.1021/je100046a
Liquid-Liquid Equilibria of Lactic Acid/Water Solutions in Trioctylamine/Dodecane/1-Dodecanol at 298.15 K: Experimental Data and Prediction:	https://www.doi.org/10.1021/acs.jced.8b00794
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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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pc:	Critical Pressure
pt:	Triple Point Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility