1-Octadecanol

Other names:

1-Hydroxyoctadecane
1-Stearyl alcohol
Adol 62
Adol 68
Aldol 62
Alfol 18
Atalco S
C18 Linear alcohol
CO 1895F
CO-1895
CO-1897
Cachalot S-43
Cachalot S-56
Conol 1675
Conol 30F
Crodacol S70
Crodacol S95NF
Crodacol-S
Decyl octyl alcohol
Dytol e-46
Kalcohl 80
Kalcohl 8098
Lanette 18 DEO
Lanol S
Lorol 28
Lorol C18
N-OCTADECYL ALCOHOL
Octadecan-1-ol
Octadecanol
Octadecanol NF
Octadecyl alcohol
Octanodecanol
Philcohol 1800
Polaax
Rita SA
Rofamol
SIPOL S
STENOL
Siponol S
Siponol SC

	Stearic alcohol
	Stearol
	Stearyl alcohol
	Stearyl alcohol NF
	Stearyl alcohol USP
	Steraffine
	Usp XIII stearyl alcohol
	Varonic BG
	n-1-Octadecanol
	n-Octadecanol
Inchi:	InChI=1S/C18H38O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h19H,2-18H2,1H
InchiKey:	GLDOVTGHNKAZLK-UHFFFAOYSA-N
Formula:	C18H38O
SMILES:	CCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	270.49
CAS:	112-92-5

Physical Properties

Property code	Value	Unit	Source
chs	-11820.00 ± 4.00	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
gf	-36.22	kJ/mol	KDB
hf	-566.90	kJ/mol	KDB
hfus	46.46	kJ/mol	Joback Method
hsub	191.20 ± 1.30	kJ/mol	NIST Webbook
hsub	187.00 ± 1.00	kJ/mol	NIST Webbook
hvap	116.80 ± 1.20	kJ/mol	NIST Webbook
log10ws	-8.40		Aqueous Solubility Prediction Method
log10ws	-8.40		Estimated Solubility Method
logp	6.240		Crippen Method
mcvol	270.350	ml/mol	McGowan Method
pc	1440.00	kPa	KDB
pt	2.93e-05 ± 1.30e-05	kPa	NIST Webbook
rinpol	2059.00		NIST Webbook
rinpol	346.29		NIST Webbook
rinpol	342.84		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2081.00		NIST Webbook

rinpol	2077.00	NIST Webbook
rinpol	2084.00	NIST Webbook
rinpol	2078.00	NIST Webbook
rinpol	2082.00	NIST Webbook
rinpol	2089.00	NIST Webbook
rinpol	2089.00	NIST Webbook
rinpol	2082.00	NIST Webbook
rinpol	2090.00	NIST Webbook
rinpol	2066.00	NIST Webbook
rinpol	2040.00	NIST Webbook
rinpol	2084.00	NIST Webbook
rinpol	2039.00	NIST Webbook
rinpol	2082.00	NIST Webbook
rinpol	2080.00	NIST Webbook
rinpol	2078.00	NIST Webbook
rinpol	2084.00	NIST Webbook
rinpol	2078.00	NIST Webbook
rinpol	345.48	NIST Webbook
rinpol	2087.70	NIST Webbook
rinpol	2067.00	NIST Webbook
rinpol	2081.00	NIST Webbook
rinpol	2066.00	NIST Webbook
rinpol	2079.00	NIST Webbook
rinpol	2080.00	NIST Webbook
rinpol	2063.00	NIST Webbook
rinpol	2085.00	NIST Webbook
rinpol	2070.00	NIST Webbook
rinpol	2071.00	NIST Webbook
rinpol	2086.00	NIST Webbook
rinpol	2084.00	NIST Webbook
rinpol	2080.00	NIST Webbook
rinpol	2084.00	NIST Webbook
rinpol	2084.00	NIST Webbook
rinpol	2084.00	NIST Webbook
rinpol	2087.00	NIST Webbook
rinpol	2087.00	NIST Webbook
rinpol	345.48	NIST Webbook
rinpol	345.48	NIST Webbook
rinpol	2074.40	NIST Webbook
rinpol	2058.00	NIST Webbook
rinpol	2067.00	NIST Webbook
rinpol	2083.00	NIST Webbook
rinpol	2089.80	NIST Webbook
rinpol	2053.00	NIST Webbook

rinpol	2059.00	NIST Webbook
rinpol	2059.00	NIST Webbook
rinpol	2074.40	NIST Webbook
rinpol	2067.80	NIST Webbook
rinpol	2095.10	NIST Webbook
rinpol	2075.00	NIST Webbook
rinpol	2074.00	NIST Webbook
rinpol	2058.00	NIST Webbook
rinpol	2065.00	NIST Webbook
rinpol	2063.00	NIST Webbook
rinpol	2064.00	NIST Webbook
rinpol	2069.00	NIST Webbook
rinpol	2067.00	NIST Webbook
rinpol	2060.00	NIST Webbook
rinpol	2061.00	NIST Webbook
rinpol	2067.00	NIST Webbook
rinpol	2050.00	NIST Webbook
rinpol	2050.00	NIST Webbook
rinpol	2081.00	NIST Webbook
rinpol	2080.00	NIST Webbook
rinpol	2082.00	NIST Webbook
rinpol	2090.00	NIST Webbook
rinpol	2084.00	NIST Webbook
rinpol	2070.00	NIST Webbook
rinpol	2082.00	NIST Webbook
rinpol	2081.00	NIST Webbook
rinpol	2059.00	NIST Webbook
rinpol	2061.00	NIST Webbook
rinpol	2061.00	NIST Webbook
rinpol	2086.00	NIST Webbook
rinpol	2089.80	NIST Webbook
rinpol	2081.00	NIST Webbook
rinpol	2070.00	NIST Webbook
rinpol	2080.00	NIST Webbook
rinpol	2079.00	NIST Webbook
ripol	2585.00	NIST Webbook
ripol	2563.00	NIST Webbook
ripol	2607.00	NIST Webbook
ripol	2534.00	NIST Webbook
ripol	2607.00	NIST Webbook
ripol	2607.00	NIST Webbook
ripol	2607.00	NIST Webbook
ripol	2607.00	NIST Webbook

ripol	2618.00		NIST Webbook
ripol	2607.00		NIST Webbook
ripol	2607.00		NIST Webbook
ripol	2581.00		NIST Webbook
ripol	2569.00		NIST Webbook
ripol	2549.00		NIST Webbook
ripol	2570.00		NIST Webbook
ripol	2558.00		NIST Webbook
ripol	2534.00		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2569.00		NIST Webbook
ripol	2544.00		NIST Webbook
ripol	2598.00		NIST Webbook
ripol	2546.00		NIST Webbook
ripol	2573.00		NIST Webbook
ripol	2574.00		NIST Webbook
ripol	2570.00		NIST Webbook
tb	608.00	K	KDB
tc	790.00	K	KDB
tf	331.60 ± 1.00	K	NIST Webbook
tf	332.65	K	Aqueous Solubility Prediction Method
tf	329.65 ± 2.00	K	NIST Webbook
tf	330.65 ± 0.25	K	NIST Webbook
tf	330.75 ± 0.60	K	NIST Webbook
tf	332.00 ± 1.50	K	NIST Webbook
tf	331.00 ± 1.50	K	NIST Webbook
tf	330.30 ± 0.40	K	NIST Webbook
tf	332.00 ± 0.25	K	NIST Webbook
tf	332.60	K	KDB
tf	331.20 ± 0.30	K	NIST Webbook
tf	331.20 ± 0.30	K	NIST Webbook
tf	331.20 ± 0.30	K	NIST Webbook
tf	331.20 ± 0.30	K	NIST Webbook
tf	330.75 ± 0.40	K	NIST Webbook
tf	328.03 ± 0.30	K	NIST Webbook
tf	328.30 ± 0.30	K	NIST Webbook
tf	331.20 ± 0.20	K	NIST Webbook
tf	331.00 ± 1.00	K	NIST Webbook

tf	325.60	K	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
tf	330.90	K	High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol
tf	331.25	K	Stearyl alcohol/palm triple pressed acid-graphite nanocomposites as phase change materials
tf	327.15	K	The manufacture of organic carbonate-poly(methyl ethylacrylate) nanowebs with thermal buffering effect
tf	331.53	K	Thermodynamics of organic mixtures containing amines. VIII. Systems with quinoline
tf	329.30	K	Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1- octadecanol, or + 1-eicosanol mixtures
tf	330.15	K	Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure
tf	331.00	K	Liquid-liquid equilibrium in binary systems of isomeric C8 aliphatic monoethers with nitromethane
tf	331.20 ± 0.30	K	NIST Webbook
tt	330.95 ± 1.00	K	NIST Webbook
tt	331.25	K	Form-stable phase change nanocomposites for thermal energy storage based on hypercrosslinked polymer nanospheres
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.56	J/mol×K	703.42	Joback Method
cpg	890.32	J/mol×K	839.60	Joback Method
cpg	875.20	J/mol×K	812.37	Joback Method
cpg	859.40	J/mol×K	785.13	Joback Method
cpg	842.87	J/mol×K	757.89	Joback Method
cpg	825.60	J/mol×K	730.66	Joback Method
cpg	904.76	J/mol×K	866.84	Joback Method
cpl	705.20	J/mol×K	343.15	NIST Webbook
dvisc	0.0003948	Pa×s	470.10	Joback Method
dvisc	0.0001646	Pa×s	528.43	Joback Method
dvisc	0.0000817	Pa×s	586.76	Joback Method
dvisc	0.0000460	Pa×s	645.09	Joback Method
dvisc	0.0000285	Pa×s	703.42	Joback Method
dvisc	0.0012130	Pa×s	411.77	Joback Method
dvisc	0.0053981	Pa×s	353.44	Joback Method
hfust	40.10	kJ/mol	330.10	NIST Webbook
hfust	40.10	kJ/mol	330.30	NIST Webbook
hfust	66.67	kJ/mol	331.20	NIST Webbook
hfust	70.08	kJ/mol	334.20	NIST Webbook
hsubt	187.40 ± 1.30	kJ/mol	323.50	NIST Webbook
hvapt	113.50	kJ/mol	345.00	NIST Webbook
hvapt	76.30	kJ/mol	536.50	NIST Webbook
hvapt	86.40	kJ/mol	469.50	NIST Webbook
hvapt	74.76	kJ/mol	608.00	KDB
pvap	1.73	kPa	483.46	Vapor-Liquid Equilibria of Binary Systems with Long-Chain Organic Compounds (Fatty Alcohol, Fatty Ester, Acylglycerol, and n-Paraffin) at Subatmospheric Pressures
rhol	812.00	kg/m3	332.00	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	487.25	K	2.05	Vapor-liquid equilibria of monoacylglicerol + monoacylglicerol or alcohol or fatty acid at subatmospheric pressures
tbp	499.04	K	3.47	Improving a variation of the DSC technique for measuring the boiling points of pure compounds at low pressures
tbrp	443.70	K	0.30	NIST Webbook
tbrp	483.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63211e+01
Coeff. B	-5.89911e+03
Coeff. C	-1.12676e+02
Temperature range (K), min.	480.15
Temperature range (K), max.	648.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.41337e+02
Coeff. B	-1.82491e+04
Coeff. C	-1.66700e+01
Coeff. D	4.33537e-07
Temperature range (K), min.	331.05
Temperature range (K), max.	777.00

Sources

Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures:	https://www.doi.org/10.1016/j.fluid.2017.03.012
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Activity Coefficients at Infinite Dilution for Hydrocarbons in Fatty Alcohols Determined by Gas-Liquid Chromatography:	https://www.doi.org/10.1021/je1005517
Improving a variation of the DSC technique for measuring the boiling points of pure compounds at low pressures:	https://www.doi.org/10.1016/j.jct.2016.04.023
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:	https://www.doi.org/10.1021/je0503857
Stearyl alcohol/palm triple pressed acid-graphite nanocomposites as phase change materials:	https://www.doi.org/10.1016/j.tca.2018.03.014
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112925&Units=SI
Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure:	https://www.doi.org/10.1016/j.fluid.2006.02.001
Measurement and Correlation of the Solid-Liquid-Gas Equilibria for Carbon Dioxide + 1-Octadecanoic Acid (Stearic Acid) and Carbon Dioxide + 1-Octadecanol (Stearyl Alcohol) Systems:	https://www.doi.org/10.1021/je9005272
Liquid-Liquid Phase Behavior of Solutions of 1-Dodecyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide ([C12mim][NTf2]) in n-Alkyl Alcohols:	https://www.doi.org/10.1021/je100359x
Thermodynamics of organic mixtures containing amines. VIII. Systems with quinoline:	https://www.doi.org/10.1016/j.jct.2008.03.015
High-Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol:	https://www.doi.org/10.1021/acs.jced.5b00330
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor-Liquid Equilibria of Binary Systems with Long-Chain Organic Compounds (Fatty Alcohol, Fatty Ester, Acylglycerol, and n-Paraffin) at Subatmospheric Pressures:	https://www.doi.org/10.1021/acs.jced.8b00168
Vapor-liquid equilibria of monoacylglicerol + monoacylglicerol or alcohol or fatty acid at subatmospheric pressures:	https://www.doi.org/10.1016/j.fluid.2017.08.013
KDB:	https://www.cheric.org/files/research/kdb/mol/mol858.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Form-stable phase change nanocomposites for thermal energy storage based on hypercrosslinked polymer nanospheres:	https://www.doi.org/10.1016/j.tca.2018.05.005
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid-Liquid Phase Behavior of Solutions of 1-Octyl- and 1-Decyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide ([C8,10mim][NTf2]) in n-Alkyl Alcohols:	https://www.doi.org/10.1021/je900988a
Liquid-liquid equilibrium in binary systems of isomeric C8 aliphatic monoethers with nitromethane:	https://www.doi.org/10.1016/j.fluid.2013.07.002
Phase equilibria of high molecular mass 1-alcohols in supercritical propane:	https://www.doi.org/10.1016/j.fluid.2007.04.027
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=858
The solid-liquid phase diagrams of binary mixtures of even saturated fatty alcohols:	https://www.doi.org/10.1016/j.fluid.2011.01.028
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The manufacture of organic carbonate-poly(methyl ethylacrylate) nanowebs with thermal buffering effect:	https://www.doi.org/10.1016/j.tca.2017.10.003

Legend

chs:	Standard solid 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

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
pc:	Critical Pressure
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume