Octadecanoic acid

Other names:

1-Heptadecanecarboxylic acid
Adeka Fatty Acid SA 910
Barolub FTA
Century 1210
Century 1220
Century 1224
Century 1230
Century 1240
Cetylacetic acid
Dar-chem 14
Edenor C18
Emersol 120
Emersol 132
Emersol 150
Emersol 153
Emersol 6349
Formula 300
Glycon DP
Glycon S-70
Glycon S-80
Glycon S-90
Glycon TP
Groco 54
Groco 55
Groco 55L
Groco 58
Groco 59
Heptadecanecarboxylic acid
Humko Industrene R
Hy-phi 1199
Hy-phi 1205
Hy-phi 1303
Hy-phi 1401
Hydrofol 1895
Hydrofol Acid 150
Hydrofol Acid 1895
Hydrofol acid 1655
Hydrofol acid 1855
Hystrene 4516
Hystrene 5016

Hystrene 7018
Hystrene 7018 FG
Hystrene 80
Hystrene 9718
Hystrene 9718 NF FG
Hystrene S-97
Hystrene T-70
Industrene 4518
Industrene 5016
Industrene 7018 FG
Industrene 8718
Industrene 9018
Industrene R
Kam 1000
Kam 2000
Kam 3000
Kiri stearic acid
Loxiol G 20
Lunac S 20
Lunac S 40
N-STEARIC ACID
NAA 173
Neo-Fat 18
Neo-Fat 18-53
Neo-Fat 18-54
Neo-Fat 18-55
Neo-Fat 18-59
Neo-Fat 18-S
Neo-fat 18-61
Octadecanoic acid (stearic acid)
PD 185
Pearl stearic
Prifac 2918
Pristerene 4904
Promulsin
Proviscol wax
SA 400 (fatty acid)
Stearex
Stearex Beads
Stearic acid
Stearophanic acid
Steric acid
Tegostearic 254

Tegostearic 255
Tegostearic 272
Tsubaki
Vanicol
Vis-Plus
WO 2 (fatty acid)
n-Octadecanoic acid
n-Octadecylic acid

Inchi: InChI=1S/C18H36O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h2-17H2,1H

InchiKey: QIQXTHQIDYTFRH-UHFFFAOYSA-N

Formula: C18H36O2

SMILES: CCCCCCCCCCCCCCCCCC(=O)O

Mol. weight [g/mol]: 284.48

CAS: 57-11-4

Physical Properties

Property code	Value	Unit	Source
chl	-11336.80 ± 2.10	kJ/mol	NIST Webbook
chl	-11280.10 ± 1.90	kJ/mol	NIST Webbook
chs	-11316.00 ± 11.00	kJ/mol	NIST Webbook
chs	-11271.00 ± 13.00	kJ/mol	NIST Webbook
chs	-11290.79	kJ/mol	NIST Webbook
chs	-11298.00	kJ/mol	NIST Webbook
gf	-165.06	kJ/mol	Joback Method
hf	-819.10 ± 5.50	kJ/mol	NIST Webbook
hfl	-947.20 ± 2.20	kJ/mol	NIST Webbook
hfs	-912.00 ± 11.00	kJ/mol	NIST Webbook
hfus	61.20	kJ/mol	Solid-Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry
hsub	204.00 ± 9.00	kJ/mol	NIST Webbook
hvap	79.09	kJ/mol	Joback Method
log10ws	-5.68		Aqueous Solubility Prediction Method
logp	6.333		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1326.58 ± 85.00	kPa	NIST Webbook
pt	4.27e-06 ± 2.00e-06	kPa	NIST Webbook
rinpol	2180.00		NIST Webbook

rinpol	2178.00	NIST Webbook
rinpol	2157.00	NIST Webbook
rinpol	2152.00	NIST Webbook
rinpol	2179.00	NIST Webbook
rinpol	2161.00	NIST Webbook
rinpol	2192.00	NIST Webbook
rinpol	2170.00	NIST Webbook
rinpol	2170.00	NIST Webbook
rinpol	2188.00	NIST Webbook
rinpol	2158.00	NIST Webbook
rinpol	2162.00	NIST Webbook
rinpol	2187.00	NIST Webbook
rinpol	2178.00	NIST Webbook
rinpol	2173.00	NIST Webbook
rinpol	2180.00	NIST Webbook
rinpol	2166.00	NIST Webbook
rinpol	2172.00	NIST Webbook
rinpol	2174.00	NIST Webbook
rinpol	2157.00	NIST Webbook
rinpol	2172.00	NIST Webbook
rinpol	2172.00	NIST Webbook
rinpol	2173.00	NIST Webbook
rinpol	2172.00	NIST Webbook
rinpol	2164.00	NIST Webbook
rinpol	2172.00	NIST Webbook
rinpol	2178.00	NIST Webbook
rinpol	2139.00	NIST Webbook
rinpol	2142.00	NIST Webbook
rinpol	2138.54	NIST Webbook
rinpol	2175.00	NIST Webbook
rinpol	2180.00	NIST Webbook
rinpol	2200.00	NIST Webbook
rinpol	2137.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2159.00	NIST Webbook
rinpol	2161.00	NIST Webbook
rinpol	2143.00	NIST Webbook
rinpol	2153.00	NIST Webbook
rinpol	2163.00	NIST Webbook
rinpol	2137.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2173.00	NIST Webbook

rinpol	2169.00	NIST Webbook
rinpol	2167.50	NIST Webbook
rinpol	2180.00	NIST Webbook
rinpol	2169.00	NIST Webbook
rinpol	2180.00	NIST Webbook
rinpol	2158.00	NIST Webbook
rinpol	2160.00	NIST Webbook
rinpol	2162.00	NIST Webbook
rinpol	2181.00	NIST Webbook
rinpol	2178.00	NIST Webbook
rinpol	2172.00	NIST Webbook
rinpol	2180.00	NIST Webbook
rinpol	2170.00	NIST Webbook
rinpol	2137.00	NIST Webbook
rinpol	2152.00	NIST Webbook
rinpol	2168.00	NIST Webbook
rinpol	2142.00	NIST Webbook
rinpol	2155.00	NIST Webbook
rinpol	2178.00	NIST Webbook
rinpol	2161.00	NIST Webbook
rinpol	2155.00	NIST Webbook
rinpol	2180.00	NIST Webbook
rinpol	2155.00	NIST Webbook
rinpol	2200.00	NIST Webbook
rinpol	2187.00	NIST Webbook
rinpol	2139.00	NIST Webbook
rinpol	2137.00	NIST Webbook
rinpol	2162.00	NIST Webbook
rinpol	2164.00	NIST Webbook
rinpol	2172.00	NIST Webbook
rinpol	2180.00	NIST Webbook
rinpol	2173.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2140.00	NIST Webbook
rinpol	2174.00	NIST Webbook
rinpol	352.98	NIST Webbook
rinpol	366.90	NIST Webbook
rinpol	350.90	NIST Webbook
rinpol	351.12	NIST Webbook
rinpol	2153.00	NIST Webbook
rinpol	2157.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	352.98	NIST Webbook
ripol	3130.00	NIST Webbook

ripol	3181.00		NIST Webbook
ripol	3136.00		NIST Webbook
ripol	3132.00		NIST Webbook
ripol	3120.00		NIST Webbook
ripol	3104.00		NIST Webbook
ripol	3181.00		NIST Webbook
ripol	3090.00		NIST Webbook
ripol	3181.00		NIST Webbook
ss	435.60	J/mol×K	NIST Webbook
tb	631.15 ± 5.00	K	NIST Webbook
tb	634.20	K	NIST Webbook
tc	805.09 ± 3.50	K	NIST Webbook
tf	326.15	K	Preparation of paraffin and fatty acid phase changing nanoemulsions for heat transfer
tf	342.90	K	Study of the Effect of Pressure on Melting Behavior of Saturated Fatty Acids in Liquid or Supercritical Carbon Dioxide
tf	327.17	K	Thermal analysis and quantitative characterization of compatibility between diflunisal and lipid excipients as raw materials for development of solid lipid nanoparticles
tf	341.55	K	Prediction of the properties of eutectic fatty acid phase change materials
tf	343.10	K	Solid Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Hexadecane
tf	341.91	K	Solid-Liquid Equilibrium of Binary Fatty Acid Mixtures
tf	342.58	K	Aqueous Solubility Prediction Method
tf	343.67	K	Measurement and PC-SAFT modeling of solid-liquid equilibrium of deep eutectic solvents of quaternary ammonium chlorides and carboxylic acids
tf	343.63	K	Solid-liquid phase equilibrium diagrams of binary mixtures containing fatty acids, fatty alcohol compounds and tripalmitin using differential scanning calorimetry

tf	343.98	K	The solid liquid phase diagrams of binary mixtures of even saturated fatty acids differing by six carbon atoms
tt	325.66	K	High latent heat stearic acid impregnated in expanded graphite
tt	344.08	K	Solubility Measurement of Lauric, Palmitic, and Stearic Acids in Ethanol, n-Propanol, and 2-Propanol Using Differential Scanning Calorimetry
tt	342.49 ± 0.02	K	NIST Webbook
tt	341.85 ± 0.50	K	NIST Webbook
tt	342.65 ± 0.01	K	NIST Webbook
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.24	J/mol×K	843.87	Joback Method
cpg	926.26	J/mol×K	930.44	Joback Method
cpg	912.95	J/mol×K	901.59	Joback Method
cpg	898.96	J/mol×K	872.73	Joback Method
cpg	835.45	J/mol×K	757.29	Joback Method
cpg	852.51	J/mol×K	786.15	Joback Method
cpg	868.77	J/mol×K	815.01	Joback Method
cps	561.90	J/mol×K	298.15	NIST Webbook
cps	501.55	J/mol×K	298.15	NIST Webbook
dvisc	0.0000381	Pa×s	698.30	Joback Method
dvisc	0.0001211	Pa×s	580.33	Joback Method
dvisc	0.0002628	Pa×s	521.34	Joback Method
dvisc	0.0024382	Pa×s	403.37	Joback Method
dvisc	0.0000245	Pa×s	757.29	Joback Method
dvisc	0.0000644	Pa×s	639.32	Joback Method
dvisc	0.0006944	Pa×s	462.36	Joback Method
hfust	64.64	kJ/mol	326.10	NIST Webbook
hfust	60.40	kJ/mol	338.30	NIST Webbook
hfust	63.20	kJ/mol	342.80	NIST Webbook
hfust	57.80	kJ/mol	344.10	NIST Webbook
hfust	50.93	kJ/mol	340.20	NIST Webbook
hfust	61.21	kJ/mol	342.50	NIST Webbook

hfust	61.30	kJ/mol	342.75	NIST Webbook
hfust	68.45	kJ/mol	342.65	NIST Webbook
hfust	61.21	kJ/mol	342.50	NIST Webbook
hsubt	158.50	kJ/mol	300.00	NIST Webbook
hsubt	158.00	kJ/mol	307.50	NIST Webbook
hsubt	166.50 ± 4.20	kJ/mol	335.50	NIST Webbook
hsubt	167.00 ± 4.20	kJ/mol	330.89	NIST Webbook
hvapt	124.30	kJ/mol	382.00	NIST Webbook
hvapt	132.60	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids
hvapt	118.90 ± 2.00	kJ/mol	377.50	NIST Webbook
hvapt	100.60	kJ/mol	553.00	NIST Webbook
hvapt	79.80	kJ/mol	515.00	NIST Webbook
pvap	8.00	kPa	548.70	Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique
pvap	1.33	kPa	501.30	Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique
pvap	9.33	kPa	553.20	Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique
pvap	6.67	kPa	543.70	Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique
pvap	5.33	kPa	535.90	Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique
pvap	4.00	kPa	528.90	Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique

pvap	2.67	kPa	519.10	Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique
sfust	1998.00	J/mol×K	342.65	NIST Webbook
sfust	198.00	J/mol×K	326.10	NIST Webbook
sfust	178.80	J/mol×K	342.75	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62589e+01
Coeff. B	-6.06525e+03
Coeff. C	-1.21641e+02
Temperature range (K), min.	501.40
Temperature range (K), max.	675.67

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.29855e+02
Coeff. B	-1.68057e+04
Coeff. C	-1.56000e+01
Coeff. D	4.06439e-06
Temperature range (K), min.	342.75
Temperature range (K), max.	799.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Solid-liquid phase equilibrium diagrams of binary mixtures containing fatty acids, fatty alcohol compounds and triacanthin using differential scanning calorimetry	https://www.doi.org/10.1016/j.fluid.2019.05.020
Solid-Liquid Equilibrium of Binary Fatty Acid Mixtures:	https://www.doi.org/10.1021/je060146z
The solid-liquid phase diagrams of binary mixtures of even saturated fatty acids differing by six carbon atoms:	https://www.doi.org/10.1016/j.tca.2009.06.018
Solubilities of Fatty Acids and Triglycerides in 1-Bromopropane:	https://www.doi.org/10.1021/je201181k
Thermal analysis and quantitative characterization of compatibility between diflunisal and lipid excipients as raw materials for development of solid lipid nanoparticles:	https://www.doi.org/10.1016/j.tca.2016.09.014

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
Measurement and Correlation of the Solid-Liquid-Gas Equilibria for Carbon Dioxide + Octadecanoic Acid (Stearic Acid) and Carbon Dioxide + 1-Octadecanol (Stearyl Alcohol) Systems:	https://www.doi.org/10.1021/je9005272
Solubilities of Hexadecanoic and Octadecanoic Acids in Supercritical CO2 With and Without Cosolvents:	https://www.doi.org/10.1021/je8007149
Apparent Molar Volumes and Viscosities of Lauric, Palmitic, and Stearic Acids in 2-Butanol at (20, 30, 40, and 60) C:	https://www.doi.org/10.1021/je025538u
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Measurement and PC-SAFT modeling of solid-liquid equilibrium of deep eutectic solvents of quaternary ammonium chlorides and carboxylic acids:	https://www.doi.org/10.1016/j.fluid.2017.04.007
Solubilities of Stearic Acid in Organic Solvents and in Azeotropic Solvent Mixtures:	https://www.doi.org/10.1021/je7006567
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Preparation of paraffin and fatty acid phase changing nanoemulsions for heat transfer:	https://www.doi.org/10.1016/j.tca.2014.12.020
Physical properties of systems of interest to the edible oil industry: Viscosities and densities of model systems formed by (triacylglycerol + fatty acid + solvent):	https://www.doi.org/10.1016/j.jct.2017.06.012
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57114&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=952
Experimental determination of the (vapor + liquid) equilibrium data of binary mixtures of fatty acids by differential scanning calorimetry:	https://www.doi.org/10.1016/j.jct.2009.07.008
Study of the Effect of Pressure on Melting Behavior of Saturated Fatty Acids in Liquid or Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je400260c
Phase Equilibria of Long-Chain Carboxylic Acids in Supercritical Propane:	https://www.doi.org/10.1021/je101077v
Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique:	https://www.doi.org/10.1016/j.tca.2012.07.034
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility Measurement of Lauric, Palmitic, and Stearic Acids in Ethanol, n-Propanol, and 2-Propanol Using Differential Scanning Calorimetry:	https://www.doi.org/10.1021/acs.jced.8b01044
Activity coefficient at infinite dilution measurements for organic solutes (polar and non-polar) in fatty compounds, Part II: C18 fatty acids:	https://www.doi.org/10.1016/j.jct.2012.12.009
Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids:	https://www.doi.org/10.1021/je300902c
Solid-Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Hexadecane:	https://www.doi.org/10.1021/acs.jced.6b00355
High latent heat stearic acid impregnated in expanded graphite:	https://www.doi.org/10.1016/j.tca.2018.03.018
Solubility and Mass Transfer Coefficient Enhancement of Stearic Acid through Hydrotropy:	https://www.doi.org/10.1021/je901041n
Solubilities of palmitic and stearic fatty acids in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.jct.2009.08.001
Prediction of the properties of eutectic fatty acid phase change materials:	https://www.doi.org/10.1016/j.tca.2017.12.024

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid 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
hfs:	Solid 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
pc:	Critical Pressure
pt:	Triple Point Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume