Octadecanoic acid, ethyl ester

Other names:	ETHYL ESTER
	ETHYL N-OCTADECANOATE
	Ethyl ocatadecanoate
	Ethyl octadecanoate
	Ethyl octadecanoate (Ethyl stearate)
	Ethyl stearate
	Radia 7185
	STEARIC ACID
	Stearic acid, ethyl ester
Inchi:	InChI=1S/C20H40O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22-4-2/h3-19
InchiKey:	MVLVMROFTAUDAG-UHFFFAOYSA-N
Formula:	C20H40O2
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	312.53
CAS:	111-61-5

Physical Properties

Property code	Value	Unit	Source
chs	-12602.20 ± 1.80	kJ/mol	NIST Webbook
gf	-116.40	kJ/mol	Joback Method
hf	-700.93	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.811		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2181.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2197.00		NIST Webbook
rinpol	2192.00		NIST Webbook

rinpol	2174.00	NIST Webbook
rinpol	2181.00	NIST Webbook
rinpol	2181.00	NIST Webbook
rinpol	2196.00	NIST Webbook
rinpol	2189.00	NIST Webbook
rinpol	2188.00	NIST Webbook
rinpol	2194.00	NIST Webbook
rinpol	2190.00	NIST Webbook
rinpol	2195.00	NIST Webbook
rinpol	2197.00	NIST Webbook
rinpol	2192.00	NIST Webbook
rinpol	2178.00	NIST Webbook
rinpol	2199.00	NIST Webbook
rinpol	2197.00	NIST Webbook
rinpol	2179.00	NIST Webbook
rinpol	2175.00	NIST Webbook
rinpol	2207.00	NIST Webbook
rinpol	2175.00	NIST Webbook
rinpol	2180.00	NIST Webbook
rinpol	2192.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2202.00	NIST Webbook
rinpol	2195.00	NIST Webbook
rinpol	2175.00	NIST Webbook
rinpol	2194.00	NIST Webbook
rinpol	2183.00	NIST Webbook
rinpol	2171.00	NIST Webbook
rinpol	2180.00	NIST Webbook
rinpol	2194.00	NIST Webbook
rinpol	2190.00	NIST Webbook
rinpol	2193.00	NIST Webbook
rinpol	2195.00	NIST Webbook
rinpol	2194.00	NIST Webbook
rinpol	2207.00	NIST Webbook
ripol	2458.00	NIST Webbook
ripol	2446.00	NIST Webbook
ripol	2444.00	NIST Webbook
ripol	2459.00	NIST Webbook
ripol	2458.00	NIST Webbook
ripol	2467.00	NIST Webbook
ripol	2429.00	NIST Webbook
ripol	2425.00	NIST Webbook
ripol	2450.00	NIST Webbook
ripol	2409.00	NIST Webbook

ripol	2467.00		NIST Webbook
ripol	2467.00		NIST Webbook
ripol	2430.00		NIST Webbook
ripol	2464.00		NIST Webbook
ripol	2483.00		NIST Webbook
ripol	2416.00		NIST Webbook
ripol	2409.00		NIST Webbook
ripol	2467.00		NIST Webbook
ripol	2455.00		NIST Webbook
ripol	2458.00		NIST Webbook
ripol	2451.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2442.00		NIST Webbook
tb	733.29	K	Joback Method
tc	904.52	K	Joback Method
tf	307.40	K	Influence of Additives (Isoamyl Laurate or Isoamyl Nonanoate) in the Solid-Liquid Equilibrium of Fatty Acid Ethyl Esters
tf	306.90 ± 0.50	K	NIST Webbook
tf	304.05 ± 0.40	K	NIST Webbook
tf	304.30 ± 1.50	K	NIST Webbook
tf	307.40	K	Solid-liquid equilibrium in ternary mixtures of ethyl laurate, ethyl palmitate and ethyl stearate
tf	307.20 ± 2.00	K	NIST Webbook
tf	306.55 ± 0.30	K	NIST Webbook
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.17	J/mol×K	904.52	Joback Method
cpg	997.86	J/mol×K	875.99	Joback Method
cpg	981.74	J/mol×K	847.45	Joback Method
cpg	964.76	J/mol×K	818.91	Joback Method
cpg	946.91	J/mol×K	790.37	Joback Method
cpg	928.17	J/mol×K	761.83	Joback Method
cpg	908.52	J/mol×K	733.29	Joback Method
dvisc	0.0021355	Pa×s	358.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters

dvisc	0.0019777	Pa×s	363.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0023132	Pa×s	353.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0025153	Pa×s	348.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0027439	Pa×s	343.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0030072	Pa×s	338.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0033073	Pa×s	333.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0050823	Pa×s	313.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0045285	Pa×s	318.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0036535	Pa×s	328.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0040574	Pa×s	323.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
hfust	59.83	kJ/mol	307.00	NIST Webbook
hsubt	161.40	kJ/mol	301.50	NIST Webbook
hvapt	109.30	kJ/mol	298.00	A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure
hvapt	111.90	kJ/mol	461.50	NIST Webbook
hvapt	106.80	kJ/mol	319.00	NIST Webbook

hvapt	92.20	kJ/mol	373.00	Express thermo-gravimetric method for the vaporization enthalpies appraisal for very low volatile molecular and ionic compounds.
pvap	4.00	kPa	512.98	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry
pvap	5.33	kPa	520.56	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry
pvap	6.67	kPa	524.45	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry
pvap	2.67	kPa	505.55	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry
pvap	1.33	kPa	490.97	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry
pvap	8.00	kPa	525.78	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry
pvap	9.33	kPa	533.97	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry

pvap	5.33	kPa	520.56	Vapor liquid equilibrium of fatty acid ethyl esters determined using DSC
rfi	1.43600		313.15	(Vapor + liquid) equilibrium for the binary systems {water + glycerol} and {ethanol + glycerol, ethyl stearate, and ethyl palmitate} at low pressures

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	487.20	K	2.00	NIST Webbook
tbrp	472.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.02510e+01
Coeff. B	-7.76715e+03
Coeff. C	-1.28730e+02
Temperature range (K), min.	517.80
Temperature range (K), max.	648.64

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.81930e+01
Coeff. B	-1.28428e+04
Coeff. C	4.76766e-03
Coeff. D	-8.25160e-09
Temperature range (K), min.	310.15

Temperature range (K), max.	328.15

Sources

Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters:	https://www.doi.org/10.1021/je100042c
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
(Vapor + liquid) equilibrium for the binary systems {water + glycerol} and {ethanol + glycerol, ethyl stearate, and ethyl palmitate} at low pressures:	https://www.doi.org/10.1016/j.jct.2011.06.016
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111615&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapor liquid equilibrium of fatty acid ethyl esters determined using DSC:	https://www.doi.org/10.1016/j.tca.2010.10.002
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1135.mol
Influence of Additives (Isoamyl Laurate or Isoamyl Nonanoate) in the Solid–Liquid Equilibrium of Fatty Acid Ethyl Esters:	https://www.doi.org/10.1021/acs.jced.8b01019
Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry:	https://www.doi.org/10.1016/j.jct.2011.01.017
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Solute Enthalpy and Vapor Pressure:	https://www.doi.org/10.1021/acs.jced.5b00444
Express the group contribution method for the vaporization enthalpies appraisal:	https://www.doi.org/10.1016/j.tca.2012.03.018
KDB, Vapor Pressure data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1135
Solid–liquid equilibrium in ternary mixtures of ethyl laurate, ethyl palmitate and ethyl stearate:	https://www.doi.org/10.1016/j.fluid.2013.08.024
(Liquid + liquid) equilibrium for the system {ethyl stearate(1) + ethanol(2) + glycerol(3)}:	https://www.doi.org/10.1016/j.jct.2011.10.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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

pvap:	Vapor pressure
rfi:	Refractive Index
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