9,12-Octadecadienoic acid (Z,Z)-, methyl ester

Other names:	(9Z,12Z)-Octadecadienoic acid methyl ester
	(Z,Z)-9,12-octadecadienoic acid methyl ester
	(Z,Z)-9,12-octadecadienoic acid, methyl ester
	9,12-Octadecadienoic acid (9Z,12Z)-, methyl ester
	9,12-Octadecadienoic acid, methyl ester, (Z,Z)
	Linoleic acid, methyl ester
	Methyl (Z,Z)-9,12-octadecadienoate
	Methyl 9-cis,12-cis-octadecadienoate
	Methyl cis,cis-9,12-octadecadienoate
	Methyl linolate
	Natural methyl linoleate
	cis-9,cis-12-Octadecadienoic acid, methyl ester
	cis-Linoleic acid methyl ester
	methyl (Z,Z)-9,12-octadecadienate
	methyl (Z,Z)-9,12-octadienoate
	methyl linoleate
Inchi:	InChI=1S/C19H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h7-8,10-
InchiKey:	WTTJVINHCBCLGX-NQLNTKRDSA-N
Formula:	C19H34O2
SMILES:	CCCCCC=CCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	294.47
CAS:	112-63-0

Physical Properties

Property code	Value	Unit	Source
chl	-11690.10 ± 1.50	kJ/mol	NIST Webbook
gf	35.62	kJ/mol	Joback Method
hf	-445.85	kJ/mol	Joback Method
hfl	-604.88	kJ/mol	NIST Webbook
hfus	48.16	kJ/mol	Joback Method
hvap	66.96	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.973		Crippen Method
mcvol	277.410	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2100.00		NIST Webbook
rinpol	2090.00		NIST Webbook

rinpol	2067.00	NIST Webbook
rinpol	2100.00	NIST Webbook
rinpol	2070.00	NIST Webbook
rinpol	2089.00	NIST Webbook
rinpol	2123.00	NIST Webbook
rinpol	2082.00	NIST Webbook
rinpol	2097.00	NIST Webbook
rinpol	2072.00	NIST Webbook
rinpol	2127.00	NIST Webbook
rinpol	2100.00	NIST Webbook
rinpol	2066.90	NIST Webbook
rinpol	2078.00	NIST Webbook
rinpol	2092.00	NIST Webbook
rinpol	2077.00	NIST Webbook
rinpol	2073.00	NIST Webbook
rinpol	2092.00	NIST Webbook
rinpol	2096.00	NIST Webbook
rinpol	2076.00	NIST Webbook
rinpol	2079.00	NIST Webbook
rinpol	2099.10	NIST Webbook
rinpol	2071.00	NIST Webbook
rinpol	2097.00	NIST Webbook
rinpol	2093.00	NIST Webbook
rinpol	2093.00	NIST Webbook
rinpol	2082.00	NIST Webbook
rinpol	2079.00	NIST Webbook
rinpol	2092.10	NIST Webbook
rinpol	2094.50	NIST Webbook
rinpol	2095.60	NIST Webbook
rinpol	2087.00	NIST Webbook
rinpol	2069.00	NIST Webbook
rinpol	2070.00	NIST Webbook
rinpol	2061.00	NIST Webbook
rinpol	2103.70	NIST Webbook
rinpol	2078.00	NIST Webbook
rinpol	2098.00	NIST Webbook
rinpol	2081.00	NIST Webbook
rinpol	2083.00	NIST Webbook
rinpol	2098.00	NIST Webbook
rinpol	2087.00	NIST Webbook
rinpol	2107.00	NIST Webbook
rinpol	2098.00	NIST Webbook
rinpol	2090.00	NIST Webbook
rinpol	2096.00	NIST Webbook

rinpol	2094.00	NIST Webbook
rinpol	2110.00	NIST Webbook
rinpol	2094.00	NIST Webbook
rinpol	2089.00	NIST Webbook
rinpol	2088.00	NIST Webbook
rinpol	2091.00	NIST Webbook
rinpol	2093.30	NIST Webbook
rinpol	2079.00	NIST Webbook
rinpol	2092.00	NIST Webbook
rinpol	2091.00	NIST Webbook
rinpol	2087.00	NIST Webbook
rinpol	2090.00	NIST Webbook
rinpol	2092.00	NIST Webbook
rinpol	2075.00	NIST Webbook
rinpol	2076.00	NIST Webbook
rinpol	2079.00	NIST Webbook
rinpol	2079.00	NIST Webbook
rinpol	2088.00	NIST Webbook
rinpol	2088.00	NIST Webbook
rinpol	2094.00	NIST Webbook
rinpol	2097.00	NIST Webbook
rinpol	2096.00	NIST Webbook
rinpol	2090.00	NIST Webbook
rinpol	2092.00	NIST Webbook
rinpol	2070.00	NIST Webbook
rinpol	2073.00	NIST Webbook
ripol	2485.00	NIST Webbook
ripol	2523.00	NIST Webbook
ripol	2483.00	NIST Webbook
ripol	2509.00	NIST Webbook
ripol	2455.00	NIST Webbook
ripol	2482.00	NIST Webbook
ripol	2502.00	NIST Webbook
ripol	2480.00	NIST Webbook
ripol	2474.00	NIST Webbook
ripol	2472.00	NIST Webbook
ripol	2472.00	NIST Webbook
ripol	2503.00	NIST Webbook
ripol	2488.00	NIST Webbook
ripol	2481.00	NIST Webbook
ripol	2484.00	NIST Webbook
ripol	2480.00	NIST Webbook
ripol	2476.00	NIST Webbook
ripol	2472.00	NIST Webbook

ripol	2513.00		NIST Webbook
ripol	2476.00		NIST Webbook
tb	718.73	K	Joback Method
tc	896.01	K	Joback Method
tf	365.89	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.45	J/mol×K	718.73	Joback Method
cpg	821.70	J/mol×K	748.28	Joback Method
cpg	839.08	J/mol×K	777.82	Joback Method
cpg	855.63	J/mol×K	807.37	Joback Method
cpg	871.40	J/mol×K	836.92	Joback Method
cpg	886.41	J/mol×K	866.47	Joback Method
cpg	900.71	J/mol×K	896.01	Joback Method
dvisc	0.0020780	Pa×s	333.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
dvisc	0.0064658	Pa×s	283.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0056550	Pa×s	288.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0049822	Pa×s	293.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0044275	Pa×s	298.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0039615	Pa×s	303.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters
dvisc	0.0035666	Pa×s	308.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters

dvisc	0.0032270	Pa×s	313.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0029358	Pa×s	318.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0026822	Pa×s	323.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0024605	Pa×s	328.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0074664	Pa×s	278.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0020934	Pa×s	338.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0019403	Pa×s	343.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0018038	Pa×s	348.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0016816	Pa×s	353.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0047980	Pa×s	293.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	
dvisc	0.0038220	Pa×s	303.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	
dvisc	0.0031660	Pa×s	313.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	
dvisc	0.0025500	Pa×s	323.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	

dvisc	0.0022660	Pa×s	333.15	Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters	
dvisc	0.0017550	Pa×s	343.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	
hvapt	107.80	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography	
speedsl	1472.00	m/s	278.15	Density and Speed of Sound Measurements on Five Fatty Acid Methyl Esters at 83 kPa and Temperatures from (278.15 to 338.15) K	
speedsl	1434.00	m/s	288.15	Density and Speed of Sound Measurements on Five Fatty Acid Methyl Esters at 83 kPa and Temperatures from (278.15 to 338.15) K	
speedsl	1398.00	m/s	298.15	Density and Speed of Sound Measurements on Five Fatty Acid Methyl Esters at 83 kPa and Temperatures from (278.15 to 338.15) K	
speedsl	1362.00	m/s	308.15	Density and Speed of Sound Measurements on Five Fatty Acid Methyl Esters at 83 kPa and Temperatures from (278.15 to 338.15) K	

speedsl	1327.00	m/s	318.15	Density and Speed of Sound Measurements on Five Fatty Acid Methyl Esters at 83 kPa and Temperatures from (278.15 to 338.15) K
speedsl	1293.00	m/s	328.15	Density and Speed of Sound Measurements on Five Fatty Acid Methyl Esters at 83 kPa and Temperatures from (278.15 to 338.15) K
speedsl	1260.00	m/s	338.15	Density and Speed of Sound Measurements on Five Fatty Acid Methyl Esters at 83 kPa and Temperatures from (278.15 to 338.15) K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	465.20	K	0.50	NIST Webbook

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
270.00	490.00	904.6
270.00	990.00	904.9
270.00	1990.00	905.4
270.00	3000.00	905.9

270.00	3990.00	906.5
270.00	5000.00	907.0
270.00	10000.00	909.6
270.00	20000.00	914.6
270.00	29990.00	919.3
270.00	39990.00	923.8
270.00	49970.00	928.2
290.00	500.00	889.7
290.00	990.00	890.0
290.00	1990.00	890.6
290.00	2990.00	891.2
290.00	3990.00	891.8
290.00	5000.00	892.4
290.00	9990.00	895.2
290.00	19990.00	900.7
290.00	30000.00	905.8
290.00	39990.00	910.7
290.00	49970.00	915.3
310.00	500.00	875.1
310.00	1000.00	875.4
310.00	1990.00	876.1
310.00	2990.00	876.7
310.00	3990.00	877.4
310.00	4990.00	878.0
310.00	9990.00	881.1
310.00	20000.00	887.0
310.00	30000.00	892.5
310.00	39990.00	897.8
310.00	49990.00	902.8
330.00	490.00	860.6
330.00	990.00	860.9
330.00	1990.00	861.6
330.00	2990.00	862.4
330.00	3990.00	863.1
330.00	4990.00	863.8
330.00	9990.00	867.1
330.00	19990.00	873.5
330.00	29980.00	879.5
330.00	39990.00	885.1
330.00	50000.00	890.4
350.00	500.00	846.2
350.00	1000.00	846.6
350.00	1990.00	847.4
350.00	2990.00	848.2

350.00	3990.00	848.9
350.00	5000.00	849.7
350.00	9990.00	853.4
350.00	19990.00	860.3
350.00	29990.00	866.7
350.00	40000.00	872.7
350.00	49980.00	878.4
370.00	490.00	831.6
370.00	990.00	832.1
370.00	1990.00	832.9
370.00	2990.00	833.8
370.00	4000.00	834.6
370.00	5000.00	835.5
370.00	10000.00	839.5
370.00	19990.00	847.0
370.00	29990.00	854.0
370.00	39990.00	860.4
370.00	49980.00	866.4
390.00	490.00	817.1
390.00	990.00	817.6
390.00	1990.00	818.5
390.00	3000.00	819.5
390.00	3990.00	820.4
390.00	4990.00	821.3
390.00	9990.00	825.8
390.00	20000.00	834.0
390.00	29990.00	841.4
390.00	40000.00	848.3
390.00	49990.00	854.7
410.00	490.00	802.5
410.00	1000.00	803.0
410.00	2000.00	804.1
410.00	2990.00	805.1
410.00	3990.00	806.2
410.00	4990.00	807.2
410.00	9990.00	812.1
410.00	19990.00	821.0
410.00	29990.00	829.1
410.00	40000.00	836.5
410.00	49970.00	843.3
430.00	490.00	787.5
430.00	1000.00	788.1
430.00	1990.00	789.3
430.00	2990.00	790.5

430.00	3990.00	791.6
430.00	5000.00	792.7
430.00	9990.00	798.1
430.00	19990.00	807.9
430.00	29990.00	816.6
430.00	40000.00	824.5
430.00	50010.00	831.8
450.00	490.00	772.5
450.00	990.00	773.2
450.00	2000.00	774.5
450.00	2990.00	775.8
450.00	4000.00	777.1
450.00	4990.00	778.3
450.00	10000.00	784.3
450.00	19990.00	794.9
450.00	30000.00	804.3
450.00	39990.00	812.8
450.00	49980.00	820.6
470.00	500.00	757.5
470.00	990.00	758.3
470.00	1990.00	759.7
470.00	3000.00	761.2
470.00	3990.00	762.6
470.00	4990.00	764.0
470.00	9990.00	770.6
470.00	19990.00	782.2
470.00	29990.00	792.4
470.00	39990.00	801.5
470.00	49980.00	809.7

Reference *https://www.doi.org/10.1021/je2008582*

Speed of sound, m/s

Pressure, kPa - Liquid	Temperature, K - Liquid	Speed of sound, m/s - Liquid
101.30	283.15	1455.0
101.30	363.15	1180.3
101.30	303.15	1382.9
101.30	383.15	1118.2
101.30	323.15	1312.6
101.30	393.15	1088.0

101.30	343.15	1245.1
10000.00	283.15	1498.2
10000.00	363.15	1237.0
10000.00	303.15	1428.9
10000.00	383.15	1178.7
10000.00	323.15	1361.4
10000.00	393.15	1150.9
10000.00	343.15	1297.9
20000.00	363.15	1288.6
20000.00	283.15	1539.0
20000.00	303.15	1472.2
20000.00	383.15	1233.8
20000.00	323.15	1407.2
20000.00	393.15	1207.3
20000.00	343.15	1346.9
30000.00	303.15	1513.6
30000.00	283.15	1577.6
30000.00	383.15	1283.1
30000.00	323.15	1450.8
30000.00	363.15	1336.6
30000.00	393.15	1258.5
30000.00	343.15	1392.6
40000.00	303.15	1552.0
40000.00	383.15	1329.0
40000.00	283.15	1614.3
40000.00	323.15	1491.3
40000.00	393.15	1304.7
40000.00	363.15	1381.1
40000.00	343.15	1435.4
50000.00	363.15	1422.6
50000.00	303.15	1588.6
50000.00	383.15	1372.3
50000.00	323.15	1530.3
50000.00	283.15	1649.2
50000.00	393.15	1348.4
50000.00	343.15	1475.1
60000.00	363.15	1462.6
60000.00	383.15	1413.2
60000.00	323.15	1567.2
60000.00	393.15	1389.4
60000.00	283.15	1682.6
60000.00	303.15	1623.5
60000.00	343.15	1513.2
70000.00	303.15	1656.3

70000.00	363.15	1500.2
70000.00	283.15	1714.0
70000.00	383.15	1452.3
70000.00	323.15	1601.4
70000.00	393.15	1428.7
70000.00	343.15	1549.4
80000.00	283.15	1745.2
80000.00	303.15	1688.3
80000.00	383.15	1489.5
80000.00	363.15	1536.1
80000.00	323.15	1634.3
80000.00	393.15	1466.7
80000.00	343.15	1583.9
90000.00	383.15	1525.2
90000.00	303.15	1719.1
90000.00	323.15	1666.2
90000.00	363.15	1570.2
90000.00	283.15	1774.4
90000.00	393.15	1503.1
90000.00	343.15	1616.7
100000.00	383.15	1558.2
100000.00	323.15	1697.2
100000.00	363.15	1602.5
100000.00	303.15	1748.7
100000.00	393.15	1537.7
100000.00	283.15	1803.2
100000.00	343.15	1648.6
110000.00	383.15	1590.3
110000.00	323.15	1726.4
110000.00	283.15	1830.9
110000.00	393.15	1570.0
110000.00	303.15	1776.9
110000.00	363.15	1634.0
110000.00	343.15	1679.0
120000.00	323.15	1754.6
120000.00	363.15	1663.9
120000.00	283.15	1857.8
120000.00	383.15	1621.1
120000.00	393.15	1600.8
120000.00	303.15	1804.4
120000.00	343.15	1708.5
130000.00	323.15	1782.4
130000.00	383.15	1650.8
130000.00	393.15	1630.7

130000.00	283.15	1884.6
130000.00	303.15	1831.3
130000.00	363.15	1693.0
130000.00	343.15	1736.1
140000.00	363.15	1720.3
140000.00	303.15	1857.0
140000.00	383.15	1679.1
140000.00	393.15	1660.1
140000.00	323.15	1808.7
140000.00	283.15	1909.9
140000.00	343.15	1763.4
150000.00	393.15	1688.0
150000.00	303.15	1883.6
150000.00	363.15	1747.4
150000.00	383.15	1707.1
150000.00	283.15	1934.7
150000.00	323.15	1834.7
150000.00	343.15	1789.7
170000.00	383.15	1759.8
170000.00	323.15	1884.5
170000.00	363.15	1799.1
170000.00	393.15	1740.7
170000.00	303.15	1932.3
170000.00	343.15	1840.9
190000.00	363.15	1847.3
190000.00	383.15	1808.6
190000.00	323.15	1931.7
190000.00	393.15	1790.0
190000.00	303.15	1979.7
190000.00	343.15	1889.3
210000.00	303.15	2023.6
210000.00	393.15	1838.1
210000.00	323.15	1977.6
210000.00	383.15	1855.8
210000.00	363.15	1894.7
210000.00	343.15	1935.4

Reference *https://www.doi.org/10.1021/je4005323*

Sources

Group Contribution Model for Predicting Viscosity of Fatty Compounds: https://www.doi.org/10.1021/je600552b

Liquid-liquid equilibria for mixtures containing water, methanol, fatty acid methyl esters, and glycerol:	https://www.doi.org/10.1016/j.fluid.2010.10.010
the vaporization enthalpies and vapor pressures of a series of unsaturated fatty acid methyl esters by correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.02.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112630&Units=SI
Speed of Sound, Density, and Derivative Properties of Methyl Oleate and Methyl Linoleate under High Pressure:	https://www.doi.org/10.1021/je4005323
Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters:	https://www.doi.org/10.1021/je100042c
Density and Speed of Sound Measurements on Five Fatty Acid Methyl Esters at 83 kPa and Temperatures from (278.15 to 338.15) K:	https://www.doi.org/10.1021/je8003854
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor liquid equilibria and densities of CO2 with four unsaturated fatty acid esters at elevated pressures:	https://www.doi.org/10.1016/j.fluid.2005.04.008
Compressed Liquid Density Measurements of Methyl Oleate and Methyl Linoleate:	https://www.doi.org/10.1021/je2008582
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid 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
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume