9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-

Other names: (Z,Z,Z)-9,12,15-Octadecatrienoic acid, methyl ester
Methyl all-cis-9,12,15-octadecatrienoate
Methyl linolenate, «alpha»
Methyl «alpha»-linolenate
[Z,Z,Z]-9,12,15-Octadecadienoic acid methyl ester
cis,cis,cis-9,12,15-Octadecatrienoic acid, methyl ester
linolenic acid, methyl ester
methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate
methyl (Z,Z,Z)-9,12,15-octadecatrienoate
methyl linolenate

Inchi: InChI=1S/C19H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h4-5,7-8

InchiKey: DVWSXZIHSUZZKJ-YSTUJMKBSA-N

Formula: C19H32O2

SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OC

Mol. weight [g/mol]: 292.46

CAS: 301-00-8

Physical Properties

Property code	Value	Unit	Source
chl	-11506.00 ± 1.50	kJ/mol	NIST Webbook
gf	115.84	kJ/mol	Joback Method
hf	-328.63	kJ/mol	Joback Method
hfl	-492.75	kJ/mol	NIST Webbook
hfus	48.36	kJ/mol	Joback Method
hvap	110.50 ± 0.50	kJ/mol	NIST Webbook
hvap	102.10	kJ/mol	NIST Webbook
log10ws	-6.20		Crippen Method
logp	5.749		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2105.40		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2073.00		NIST Webbook

rinpol	2069.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2081.00		NIST Webbook
rinpol	2089.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2081.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2092.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2081.00		NIST Webbook
rinpol	2071.80		NIST Webbook
rinpol	2099.00		NIST Webbook
ripol	2550.00		NIST Webbook
ripol	2558.00		NIST Webbook
ripol	2590.00		NIST Webbook
ripol	2583.00		NIST Webbook
ripol	2583.00		NIST Webbook
ripol	2508.00		NIST Webbook
ripol	2590.00		NIST Webbook
tb	722.89	K	Joback Method
tc	904.64	K	Joback Method
tf	360.81	K	Joback Method

vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.46	J/mol×K	722.89	Joback Method
cpg	875.18	J/mol×K	904.64	Joback Method
cpg	861.21	J/mol×K	874.35	Joback Method
cpg	846.59	J/mol×K	844.06	Joback Method
cpg	815.15	J/mol×K	783.47	Joback Method
cpg	831.25	J/mol×K	813.77	Joback Method
cpg	798.24	J/mol×K	753.18	Joback Method
dvisc	0.0014021	Pa×s	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0033010	Pa×s	303.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
dvisc	0.0027900	Pa×s	313.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
dvisc	0.0040220	Pa×s	293.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
dvisc	0.0022990	Pa×s	323.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
dvisc	0.0018620	Pa×s	333.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds

dvisc	0.0015960	Pa×s	343.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	
dvisc	0.0063612	Pa×s	278.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0056183	Pa×s	283.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0050032	Pa×s	288.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0044844	Pa×s	293.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0040429	Pa×s	298.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0036665	Pa×s	303.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0033405	Pa×s	308.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0012527	Pa×s	373.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	

dvisc	0.0026750	Pa×s	318.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0024725	Pa×s	323.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0023030	Pa×s	328.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0021234	Pa×s	333.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0019659	Pa×s	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0018165	Pa×s	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0016878	Pa×s	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0015827	Pa×s	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0014877	Pa×s	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0029253	Pa×s	313.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0013272	Pa×s	368.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
hvapt	87.70	kJ/mol	426.50	NIST Webbook
hvapt	110.50	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography
speedsl	1272.00	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
speedsl	1340.00	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	1375.00	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	1411.00	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	1448.00	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	1485.00	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	1306.00	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	455.20	K	0.40	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C301008&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.02.008
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel:	https://www.doi.org/10.1021/je1012235
Group Contribution Model for Predicting Viscosity of Fatty Compounds:	https://www.doi.org/10.1021/je600552b

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
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