

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:	DVWSXZIH SUZZKJ-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	2078.00		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	2084.00		NIST Webbook

rinpol	2078.00		NIST Webbook
rinpol	2105.40		NIST Webbook
rinpol	2089.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2081.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2081.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2125.00		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	2081.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2071.80		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2092.00		NIST Webbook
rinpol	2073.00		NIST Webbook
ripol	2583.00		NIST Webbook
ripol	2583.00		NIST Webbook
ripol	2550.00		NIST Webbook
ripol	2508.00		NIST Webbook
ripol	2590.00		NIST Webbook
ripol	2590.00		NIST Webbook
ripol	2558.00		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
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.46	J/molxK	722.89	Joback Method
cpg	815.15	J/molxK	783.47	Joback Method
cpg	831.25	J/molxK	813.77	Joback Method
cpg	846.59	J/molxK	844.06	Joback Method
cpg	861.21	J/molxK	874.35	Joback Method
cpg	875.18	J/molxK	904.64	Joback Method
cpg	798.24	J/molxK	753.18	Joback Method
dvisc	0.0029253	Paxs	313.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0026750	Paxs	318.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0024725	Paxs	323.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0023030	Paxs	328.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0021234	Paxs	333.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0019659	Paxs	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0018165	Paxs	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0016878	Paxs	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0033405	Paxs	308.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0014877	Paxs	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0014021	Paxs	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0013272	Paxs	368.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0012527	Paxs	373.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0040220	Paxs	293.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds

dvisc	0.0036665	Paxs	303.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0027900	Paxs	313.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	
dvisc	0.0022990	Paxs	323.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	
dvisc	0.0018620	Paxs	333.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	
dvisc	0.0015960	Paxs	343.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds	
dvisc	0.0040429	Paxs	298.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0044844	Paxs	293.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0050032	Paxs	288.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0056183	Paxs	283.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	

dvisc	0.0015827	Paxs	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0033010	Paxs	303.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
dvisc	0.0063612	Paxs	278.15	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 enthalpies and vapor pressures of a series of unstaured fatty acid methyl esters by correlation gas chromatography
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	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
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	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

Pressure Dependent Properties

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

Sources

Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters
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/je1012235>
<https://www.doi.org/10.1021/je8003854>
<http://link.springer.com/article/10.1007/BF02311772>

Group Contribution Model for Predicting Viscosity of Fatty Compounds
the vaporization enthalpies and vapor pressures of a series of unsaturated fatty acid methyl esters by correlation gas chromatography:
NIST Webbook:

<https://www.doi.org/10.1021/je600552b>

<https://www.doi.org/10.1016/j.tca.2007.02.008>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C301008&Units=SI>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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

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