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

Other names:	(Z,Z)-9,12-Octadecadienoic acid
	(Z,Z)-Octadeca-9, 12-dienoic acid
	9,12-Linoleic acid
	9,12-OCTADECADIENOIC ACID
	9,12-Octadecadienoic acid (9Z,12Z)-
	9,12-Octadecadienoic acid, cis,cis-
	9-(Z), 12-(Z)-Octadecadienoic acid
	9-cis,12-cis-Linoleic acid
	9Z,12Z-Linoleic acid
	Acide linoleique
	CIS,CIS-9,12-OCTADECADIENOIC ACID
	Emersol 310
	Emersol 315
	Extra Linoleic 90
	Grape seed oil
	LINOLEIC ACID
	Leinoleic acid
	Linoleic
	Linolic acid
	Octadeca-9,12-dienoic acid, (cis,cis)-
	Polylin 515
	Polylin No. 515
	TELFAIRIC ACID
	Unifac 6550
	Vespula pensylvanica b708568k063
	all-cis-9,12-Octadecadienoic acid
	cis,cis-Linoleic acid
	cis-9,cis-12-Octadecadienoic acid
	cis-«DELTA»9,12-Octadecadienoic acid
	cis-Â«DELTAÂ»9,12-Octadecadienoic acid
Inchi:	InChI=1S/C18H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h6-7,9-10H,
InchiKey:	OYHQOLUKZRVURQ-HZJYTTRNSA-N
Formula:	C18H32O2
SMILES:	CCCCCC=CCC=CCCCCCCCC(=O)O
Mol. weight [g/mol]:	280.45
CAS:	60-33-3

Physical Properties

Property code	Value	Unit	Source
gf	-4.62	kJ/mol	Joback Method
hf	-445.22	kJ/mol	Joback Method
hfl	-634.70	kJ/mol	NIST Webbook
hfus	48.47	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.885		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2156.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2133.00		NIST Webbook
rinpol	2144.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2154.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2095.20		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	2144.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2173.00		NIST Webbook
rinpol	2156.00		NIST Webbook
rinpol	2126.00		NIST Webbook
rinpol	2159.00		NIST Webbook
rinpol	2114.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2113.00		NIST Webbook

rinpol	2113.00	NIST Webbook
rinpol	2106.00	NIST Webbook
rinpol	2112.00	NIST Webbook
rinpol	2145.80	NIST Webbook
rinpol	2179.00	NIST Webbook
rinpol	2113.00	NIST Webbook
rinpol	2147.00	NIST Webbook
rinpol	2128.00	NIST Webbook
rinpol	2136.00	NIST Webbook
rinpol	2130.00	NIST Webbook
rinpol	2109.00	NIST Webbook
rinpol	2135.00	NIST Webbook
rinpol	2136.00	NIST Webbook
rinpol	2113.00	NIST Webbook
rinpol	2154.00	NIST Webbook
rinpol	2111.00	NIST Webbook
rinpol	2130.00	NIST Webbook
rinpol	2146.00	NIST Webbook
rinpol	2144.00	NIST Webbook
rinpol	2156.00	NIST Webbook
rinpol	2136.00	NIST Webbook
rinpol	2122.00	NIST Webbook
rinpol	2156.00	NIST Webbook
rinpol	2132.00	NIST Webbook
rinpol	2150.00	NIST Webbook
rinpol	2107.00	NIST Webbook
rinpol	2128.00	NIST Webbook
rinpol	2130.00	NIST Webbook
rinpol	2131.00	NIST Webbook
rinpol	2140.00	NIST Webbook
rinpol	2123.00	NIST Webbook
rinpol	2123.00	NIST Webbook
rinpol	2119.00	NIST Webbook
rinpol	2107.00	NIST Webbook
rinpol	2125.00	NIST Webbook
rinpol	2125.00	NIST Webbook
rinpol	2130.00	NIST Webbook
rinpol	2104.00	NIST Webbook
rinpol	2097.00	NIST Webbook
rinpol	2125.00	NIST Webbook
rinpol	2130.00	NIST Webbook
rinpol	2152.00	NIST Webbook
rinpol	2105.00	NIST Webbook
ripol	3157.00	NIST Webbook

ripol	3215.00		NIST Webbook
ripol	3168.00		NIST Webbook
ripol	3157.00		NIST Webbook
ripol	3157.00		NIST Webbook
ripol	3176.00		NIST Webbook
ripol	3160.00		NIST Webbook
tb	765.61	K	Joback Method
tc	944.34	K	Joback Method
tf	268.20	K	Solid-Liquid Equilibria in Fatty Acid/Triglycerol Systems
tf	267.83	K	Solid Liquid Equilibrium of Binary Mixtures Containing Fatty Acids and Triacylglycerols
tf	266.40 ± 0.80	K	NIST Webbook
tf	266.20 ± 1.00	K	NIST Webbook
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.21	J/mol×K	944.34	Joback Method
cpg	787.02	J/mol×K	765.61	Joback Method
cpg	802.93	J/mol×K	795.40	Joback Method
cpg	818.10	J/mol×K	825.19	Joback Method
cpg	832.56	J/mol×K	854.97	Joback Method
cpg	846.37	J/mol×K	884.76	Joback Method
cpg	859.57	J/mol×K	914.55	Joback Method
dvisc	0.0000180	Pa×s	765.61	Joback Method
dvisc	0.0023129	Pa×s	393.21	Joback Method
dvisc	0.0005934	Pa×s	455.28	Joback Method
dvisc	0.0002110	Pa×s	517.34	Joback Method
dvisc	0.0000937	Pa×s	579.41	Joback Method
dvisc	0.0000486	Pa×s	641.48	Joback Method
dvisc	0.0000284	Pa×s	703.54	Joback Method
hfust	47.70	kJ/mol	303.00	NIST Webbook
hvapt	134.10	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	502.70	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60422e+01
Coeff. B	-6.13615e+03
Coeff. C	-9.91760e+01
Temperature range (K), min.	489.15
Temperature range (K), max.	671.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.48236e+02
Coeff. B	-1.87631e+04
Coeff. C	-1.78156e+01
Coeff. D	2.59652e-06
Temperature range (K), min.	268.15
Temperature range (K), max.	628.00

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=984
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid-Liquid Equilibria in Fatty Acid/Triglycerol Systems:	https://www.doi.org/10.1021/je101092j
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=984
Phase equilibrium measurements of ternary systems formed by linoleic and linolenic acids in carbon dioxide/ethanol mixtures:	https://www.doi.org/10.1016/j.jct.2009.05.012
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Viscosities of Fatty Mixtures: Experimental Data and Prediction:	https://www.doi.org/10.1021/je700293s
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solid Liquid Equilibrium of Binary Mixtures Containing Fatty Acids and Triacylglycerols:	https://www.doi.org/10.1021/je200033b
Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids:	https://www.doi.org/10.1021/je300902c
Measurements of Binary Diffusion Coefficient and Partition Ratio at Infinite Dilution for Linoleic Acid and Carbon Dioxide:	https://www.doi.org/10.1021/je020205i
Activity coefficient at infinite dilution measurements for organic solutes in the omega-3 polyunsaturated fatty ester ethyl stearidonate:	https://www.doi.org/10.1016/j.jct.2012.12.009
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
hfust:	Enthalpy of fusion 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
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