Triolein

Other names:	1,2,3-propanetriyl trioleate 1,2,3-tri(cis-9-octadecenoyl)glycerol 2,3-Bis[(9Z)-9-octadecenoyloxy]propyl (9Z)-9-octadecenoate 9-Octadecenoic acid (9Z)-, 1,1',1''-(1,2,3-propanetriyl) ester 9-Octadecenoic acid (9Z)-, 1,2,3-propanetriyl ester 9-Octadecenoic acid 1,2,3-propanetriyl ester, (Z)- 9-octadecenoic acid (Z)-, 1,2,3-propanetriyl ester Aldo TO Emerest 2423 Emery 2423 Emery oleic acid ester 2230 Glycerin trioleate Glycerol triolein Kemester 1000 Oleic triglyceride Olein, tri- Priolube 1435 Radia 7363 Raoline Trioleoylglyceride glycerol trioleate glyceryl trioleate glyceryl tris[(Z)-9-octadecenoate] glyceryl-1,2,3-trioleate oleic acid triglyceride oleyl triglyceride trioleoylglycerol
Inchi:	InChI=1S/C57H104O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-55(58)61-52-
InchiKey:	PHYFQTYBJUILEZ-IUPFWZBJSA-N
Formula:	C57H104O6
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OCC(COC(=O)CCCCCCCC=CCCCCCCCC)OC(=O)C
Mol. weight [g/mol]:	885.43
CAS:	122-32-7

Physical Properties

Property code	Value	Unit	Source

chl	-35099.60 ± 1.30	kJ/mol	NIST Webbook
gf	-34.48	kJ/mol	Joback Method
hf	-1607.83	kJ/mol	Joback Method
hfus	148.83	kJ/mol	Joback Method
hvap	169.43	kJ/mol	Joback Method
log10ws	-19.94		Crippen Method
logp	18.097		Crippen Method
mcvol	823.410	ml/mol	McGowan Method
pc	245.06	kPa	Joback Method
tb	1744.47	K	Joback Method
tc	4418.33	K	Joback Method
tf	268.20	K	Solid-Liquid Equilibria in Fatty Acid/Triglycerol Systems
tf	279.22	K	Solid Liquid Equilibrium of Binary Mixtures Containing Fatty Acids and Triacylglycerols
vc	3.233	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3418.56	J/mol×K	1744.47	Joback Method
cpg	3789.05	J/mol×K	2190.11	Joback Method
cpg	4601.71	J/mol×K	2635.76	Joback Method
cpg	6184.33	J/mol×K	3081.40	Joback Method
cpg	8864.70	J/mol×K	3527.04	Joback Method
cpg	12970.60	J/mol×K	3972.68	Joback Method
cpg	18829.83	J/mol×K	4418.33	Joback Method
dvisc	0.0000014	Pa×s	918.39	Joback Method
dvisc	0.0000006	Pa×s	1056.07	Joback Method
dvisc	0.0000003	Pa×s	1193.75	Joback Method
dvisc	0.0000001	Pa×s	1331.43	Joback Method
dvisc	9.1401528e-08	Pa×s	1469.11	Joback Method
dvisc	6.1659533e-08	Pa×s	1606.79	Joback Method
dvisc	4.4262050e-08	Pa×s	1744.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122327&Units=SI
Phase equilibria of methanol triolein system at elevated temperature and pressure:	https://www.doi.org/10.1016/j.fluid.2005.10.010
Effect of triolein addition of the solubility of capsanthin in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.jct.2012.02.030
Viscosities of Fatty Mixtures: Experimental Data and Prediction:	https://www.doi.org/10.1021/je700293s
Physical properties of systems of interest to the edible oil industry:	https://www.doi.org/10.1016/j.jct.2017.06.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Viscosities and densities of model systems formed by (triacylglycerol + fatty acid + solvent):	https://en.wikipedia.org/wiki/Joback_method
Joback Method:	https://www.doi.org/10.1016/j.fluid.2013.11.006
Hydrogen solubility in triolein, and propane solubility in oleic acid for second generation BDF synthesis by use of hydrodeoxygenation reaction:	https://www.doi.org/10.1021/je101092j
Solid-Liquid Equilibria in Fatty Acid/Triglycerol Systems: Phase Equilibrium of Biodiesel Compounds for the Triolein + Palmitic Acid + Methanol System with Dimethyl Ether as Cosolvent:	https://www.doi.org/10.1021/je700711n
Solid-Liquid Equilibrium of Binary Mixtures Containing Fatty Acids and Triacylglycerols:	https://www.doi.org/10.1021/je200033b
Phase Equilibria of Glycerol Tristearate and Glycerol Trioleate in Carbon Dioxide and Sulfur Hexafluoride:	https://www.doi.org/10.1021/je300801j
Solubility of b-carotene in ethanol- and triolein-modified CO2:	https://www.doi.org/10.1016/j.jct.2011.07.013
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Phase equilibria of triolein to biodiesel reactor systems:	https://www.doi.org/10.1016/j.fluid.2015.09.049
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of .beta.-Carotene and Glyceryl Trioleate Mixture in Supercritical CO2:	https://www.doi.org/10.1021/je400553y

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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume