Trilinolein

Other names:	9,12-Octadecadienoic acid (Z,Z)-, 1,2,3-propanetriyl ester propane-1,2,3-triyl tris[(9Z,12Z)-octadeca-9,12-dienoate]
Inchi:	InChI=1S/C57H98O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-55(58)61-52-5
InchiKey:	HBOQXIRUPVQLKX-BBWANDEASA-N
Formula:	C57H98O6
SMILES:	CCCCCC=CCC=CCCCCCCCC(=O)OCC(COC(=O)CCCCCCCC=CCC=CCCCCC)OC(=
Mol. weight [g/mol]:	879.38
CAS:	537-40-6

Physical Properties

Property code	Value	Unit	Source
chl	-34555.70 ± 1.30	kJ/mol	NIST Webbook
gf	206.18	kJ/mol	Joback Method
hf	-1256.17	kJ/mol	Joback Method
hfus	149.44	kJ/mol	Joback Method
hvap	169.30	kJ/mol	Joback Method
log10ws	-19.50		Crippen Method
logp	17.425		Crippen Method
mcvol	810.510	ml/mol	McGowan Method
pc	257.48	kPa	Joback Method
tb	1756.95	K	Joback Method
tc	3990.34	K	Joback Method
tf	256.00	K	Solid-Liquid Equilibria in Fatty Acid/Triglycerol Systems
vc	3.174	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3483.90	J/mol×K	1756.95	Joback Method
cpg	4037.71	J/mol×K	2129.18	Joback Method
cpg	5050.78	J/mol×K	2501.41	Joback Method
cpg	6758.13	J/mol×K	2873.64	Joback Method

cpg	9394.79	J/mol×K	3245.87	Joback Method
cpg	13195.76	J/mol×K	3618.10	Joback Method
cpg	18396.07	J/mol×K	3990.34	Joback Method
dvisc	0.0000012	Pa×s	903.15	Joback Method
dvisc	0.0000004	Pa×s	1045.45	Joback Method
dvisc	0.0000002	Pa×s	1187.75	Joback Method
dvisc	0.0000001	Pa×s	1330.05	Joback Method
dvisc	6.6147480e-08	Pa×s	1472.35	Joback Method
dvisc	4.4353058e-08	Pa×s	1614.65	Joback Method
dvisc	3.1728738e-08	Pa×s	1756.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C537406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Solid-Liquid Equilibria in Fatty Acid/Triglycerol Systems: Experimental Data and Prediction:	https://www.doi.org/10.1021/je101092j
Viscosities of Fatty Mixtures:	https://www.doi.org/10.1021/je700293s
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
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

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