Tristearin

Other names:	1,2,3-Propanetriyl trioctadecanoate
	1,2,3-propanetriyl tri(octadecanoate)
	Dynasan 118
	Glycowax S 932
	Hardened oil
	Octadecanoic acid, 1,1',1''-(1,2,3-propanetriyl) ester
	Spezialfett 118
	Stearic triglyceride
	Stearin
	Stearoyl triglyceride
	Trioctadecanoin
	glycerol trioctadecanoate
	glycerol tristearate
	glyceryl tristearate
	octadecanoic acid, 1,2,3-propanetriyl ester
	stearic acid triglyceride
	stearic acid triglycerin ester
	stearin, tri-
Inchi:	InChI=1S/C57H110O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-55(58)61-52-
InchiKey:	DCXXMTOCNZCJGO-UHFFFAOYSA-N
Formula:	C57H110O6
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCCCC)OC(=O)CC
Mol. weight [g/mol]:	891.48
CAS:	555-43-1

Physical Properties

Property code	Value	Unit	Source
chs	-35806.70 ± 1.80	kJ/mol	NIST Webbook
gf	-275.14	kJ/mol	Joback Method
hf	-1959.49	kJ/mol	Joback Method
hfus	197.55	kJ/mol	Thermal Properties of Tristearin by Adiabatic and Differential Scanning Calorimetry
hfus	115.71	kJ/mol	Measurement and modelling of binary (solid + liquid + vapour) equilibria involving lipids and CO2
hvap	236.20 ± 8.30	kJ/mol	NIST Webbook

log10ws	-20.38		Crippen Method
logp	18.769		Crippen Method
mcvol	836.310	ml/mol	McGowan Method
pc	233.51	kPa	Joback Method
sl	1534.70	J/mol×K	NIST Webbook
tb	1731.99	K	Joback Method
tc	4994.80	K	Joback Method
tf	346.60	K	Solid Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Hexadecane
tf	345.75	K	Solid Liquid Equilibrium of Binary Mixtures Containing Fatty Acids and Triacylglycerols
tf	330.00 ± 1.00	K	NIST Webbook
tf	344.60 ± 2.00	K	NIST Webbook
tt	345.70 ± 0.20	K	NIST Webbook
tt	327.20 ± 0.20	K	NIST Webbook
tt	328.30 ± 1.00	K	NIST Webbook
tt	346.30 ± 1.00	K	NIST Webbook
tt	336.70 ± 1.00	K	NIST Webbook
vc	3.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	17839.21	J/mol×K	4994.80	Joback Method
cpg	3365.32	J/mol×K	1731.99	Joback Method
cpg	11554.09	J/mol×K	4451.00	Joback Method
cpg	7429.29	J/mol×K	3907.19	Joback Method
cpg	5006.40	J/mol×K	3363.39	Joback Method
cpg	3827.04	J/mol×K	2819.59	Joback Method
cpg	3432.81	J/mol×K	2275.79	Joback Method
cpl	1969.00	J/mol×K	346.50	NIST Webbook
cpl	1975.00	J/mol×K	353.00	NIST Webbook
dvisc	0.0000002	Pa×s	1332.81	Joback Method
dvisc	6.1803902e-08	Pa×s	1731.99	Joback Method
dvisc	0.0000007	Pa×s	1066.69	Joback Method
dvisc	0.0000018	Pa×s	933.63	Joback Method
dvisc	8.5769412e-08	Pa×s	1598.93	Joback Method
dvisc	0.0000001	Pa×s	1465.87	Joback Method

dvisc	0.0000004	Pa×s	1199.75	Joback Method
hfust	203.26	kJ/mol	345.70	NIST Webbook
hfust	203.26	kJ/mol	345.70	NIST Webbook
hvapt	174.90	kJ/mol	506.00	NIST Webbook
hvapt	167.50	kJ/mol	554.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid Liquid Equilibrium of Binary Mixtures Containing Fatty Acids and Triacylglycerols:	https://www.doi.org/10.1021/je200033b
Thermal Properties of Tristearin by Adiabatic and Differential Scanning Calorimetry:	https://www.doi.org/10.1021/je050092d
Solid-Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12:0-C18) + Heptane:	https://www.doi.org/10.1021/acs.jced.6b00355
Solubilities of Fatty Acids and Triglycerides in 1-Bromopropane:	https://www.doi.org/10.1021/je201181k
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C555431&Units=SI
Phase Equilibria of Glycerol Tristearate and Glycerol Trioleate in Carbon Dioxide and Sulfur Hexafluoride:	https://www.doi.org/10.1021/je300801j
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurement and modelling of binary (solid + liquid + vapour) equilibria involving lipids and CO2:	https://www.doi.org/10.1016/j.jct.2013.10.007

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume