Tripalmitin

Other names:	1,2,3-propanetriyl tri(hexadecanoate) Barolub Dynasan 116 GLYCEROL TRIPALMITATE GLYCERYL TRIPALMITATE Hexadecanoic acid, 1,1',1''-(1,2,3-propanetriyl) ester Hexadecanoic acid, 1,2,3-propanetriyl ester Palmitic acid triglycerin ester Palmitic triglyceride Palmitin, tri- Spezialfett 116 TRIPALMITOYLGLYCEROL Triglyceryl palmitate Tripalmitate glycerin tripalmitate hexadecanoic acid 1,2,3-propanetriyl ester triglyceride PPP
Inchi:	InChI=1S/C51H98O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-49(52)55-46-48(57-5
InchiKey:	PVNIQBQSYATKKL-UHFFFAOYSA-N
Formula:	C51H98O6
SMILES:	CCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCC)OC(=O)CCCCCC
Mol. weight [g/mol]:	807.32
CAS:	555-44-2

Physical Properties

Property code	Value	Unit	Source
chs	-31605.90 ± 1.80	kJ/mol	NIST Webbook
gf	-325.66	kJ/mol	Joback Method
hf	-1835.65	kJ/mol	Joback Method
hfus	121.00	kJ/mol	Binary solid liquid gas equilibrium of the tripalmitin/CO2 and ubiquinone/CO2 systems
hvap	217.10 ± 7.60	kJ/mol	NIST Webbook
log10ws	-17.87		Crippen Method
logp	16.429		Crippen Method
mcvol	751.770	ml/mol	McGowan Method
pc	280.76	kPa	Joback Method

sl	1387.40	J/mol×K	NIST Webbook
tb	1594.71	K	Joback Method
tc	3258.54	K	Joback Method
tf	338.80 ± 2.00	K	NIST Webbook
tf	339.40 ± 0.70	K	NIST Webbook
tf	337.95	K	KDB
tf	339.44	K	Solid-liquid phase equilibrium diagrams of binary mixtures containing fatty acids, fatty alcohol compounds and tripalmitin using differential scanning calorimetry
tf	340.70	K	Solid Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Hexadecane
tf	339.00	K	Solid-Liquid Equilibria in Fatty Acid/Triglycerol Systems
tf	338.82	K	Solid Liquid Equilibrium of Binary Mixtures Containing Fatty Acids and Triacylglycerols
tt	338.90 ± 0.20	K	NIST Webbook
tt	339.50 ± 1.00	K	NIST Webbook
tt	329.30 ± 1.00	K	NIST Webbook
tt	317.90 ± 0.20	K	NIST Webbook
tt	318.40 ± 1.00	K	NIST Webbook
vc	2.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2984.01	J/mol×K	2149.32	Joback Method
cpg	2982.50	J/mol×K	1594.71	Joback Method
cpg	3013.89	J/mol×K	2426.63	Joback Method
cpg	3132.06	J/mol×K	2703.93	Joback Method
cpg	3390.16	J/mol×K	2981.24	Joback Method
cpg	3839.85	J/mol×K	3258.54	Joback Method
cpg	2990.76	J/mol×K	1872.02	Joback Method
cpl	1665.00	J/mol×K	343.00	NIST Webbook
cpl	1753.10	J/mol×K	338.80	NIST Webbook
dvisc	0.0000002	Pa×s	1594.71	Joback Method
dvisc	0.0000004	Pa×s	1351.81	Joback Method

dvisc	0.0000006	Pa×s	1230.36	Joback Method
dvisc	0.0000010	Pa×s	1108.91	Joback Method
dvisc	0.0000020	Pa×s	987.46	Joback Method
dvisc	0.0000003	Pa×s	1473.26	Joback Method
dvisc	0.0000049	Pa×s	866.01	Joback Method
hfust	179.37	kJ/mol	338.90	NIST Webbook
hfust	179.37	kJ/mol	338.90	NIST Webbook
hfust	121.00	kJ/mol	337.40	NIST Webbook
hfust	162.60	kJ/mol	340.50	NIST Webbook
hvapt	160.80	kJ/mol	539.00	NIST Webbook
hvapt	166.30	kJ/mol	483.00	NIST Webbook

Sources

Binary solid liquid gas equilibrium of the tripalmitin/CO2 and tristearin/CO2 systems:	https://www.doi.org/10.1016/j.fluid.2005.12.017
Solid-Liquid Equilibria in Fatty Acid/Triglycerol Systems:	https://www.doi.org/10.1021/je101092j
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C555442&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1139.mol
Solid Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Tetradecane:	https://www.doi.org/10.1021/acs.jced.6b00355
Solid-Liquid Equilibrium of Binary Mixtures Containing Fatty Acids and Triacylglycerols:	https://www.doi.org/10.1021/je200033b
Solubilities of Fatty Acids and Triglycerides in 1-Bromopropane:	https://www.doi.org/10.1021/je201181k
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Physical properties of systems of interest to the edible oil industry: Crippen Method:	https://www.doi.org/10.1016/j.jct.2017.06.012
Viscosities and densities of model systems formed by (triacylglycerol + fatty acid + solvent):	https://www.chemeo.com/doc/models/crippen_log10ws
Solid-liquid phase equilibrium diagrams of binary mixtures containing fatty acids, fatty alcohol compounds and tripalmitin using differential scanning calorimetry:	https://www.doi.org/10.1016/j.fluid.2019.05.020

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